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Computer simulation of plant operation for use in process operator training

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COMPUTER SIMULATION OF PLANT OPERATION

FOR USE IN

PROCESS OPERATOR TRAINING

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Summary

The application of microcomputer-based simulation of chemical plant operation for the training of process plant personnel was studied.

The use of small scale, relatively low cost microcomputer-based simulations was demonstrated and their value in satisfying plant personnel training needs was established.

The role and training of the process operator are surveyed together with the use of simulation in training within the process industries. Computer-based-training and in particular microcomputer-based simulation training are proposed as a highly suitable medium for training plant personnel.

A number of methods of simulating chemical plant operation to achieve process personnel training objectives on microcomputers have been developed and several examples of both generic and plant-specfic training simulations are presented.

Chapter 1 Introduction

The operation of any process plant is a marriage between the process and control equipment and the operating personnel as shown in Figure 1.1. The efficiency of the process operators has a significant effect on the overall plant efficiency. The process operators require sufficient plant knowledge to monitor and operate the plant safely under normal conditions so that the required production is obtained at minimal cost. When abnormal conditions occur such as in the failure of plant equipment, the operators require operating skills such as fault detection and diagnosis so that the failure can be identified quickly and its effect on production minimised. A lack of operator knowledge and skill can lead to inefficient plant operation, unsafe working practices and catastrophic events such as the recent Chernobyl Nuclear Power Station disaster(C10).

Process plants are increasingly becoming more automated requiring little or no operator intervention. The frequency of plant start-up and shutdown has been reduced due to improved reliability of equipment and thus process operators have fewer experiences of abnormal plant operation. I.C.I.'s Severnside Works discovered that under normal operating conditions day-to-day running caused few problems. However, when abnormal or emergency conditions arose such as in the severe winter of 1981/82, the response of the operators in coping with the problems in a predictable and correct manner pointed to the need for a higher level of performance(B12).

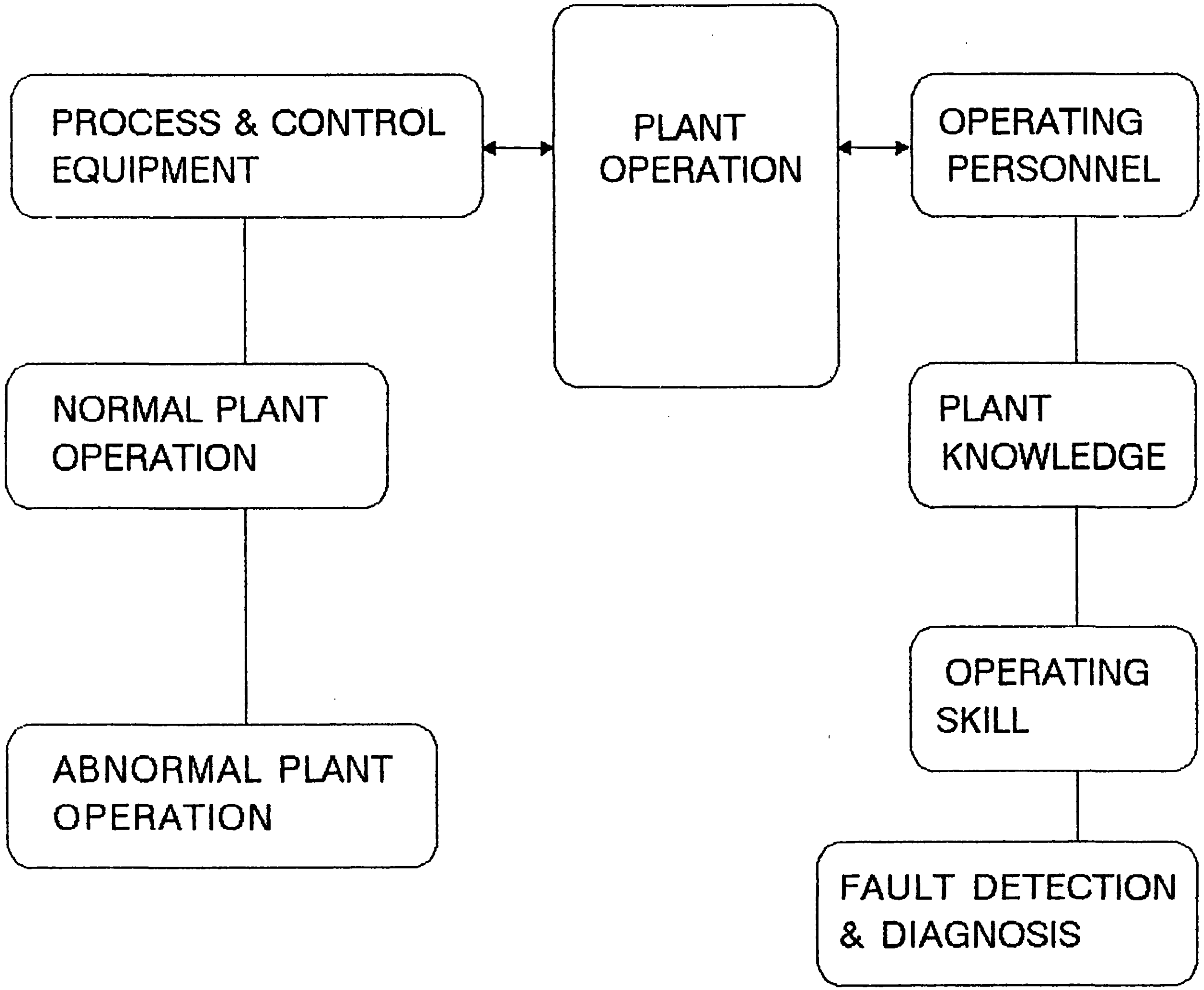


Figure 1.1 : Plant Operation

Computer simulation has been used in the process industries for many years as an aid for the design and analysis of process systems. The value of simulation is well established. Simulators have also been used for training process operating personnel, however their use has been restricted by the relatively high cost involved. More recently, the widespread availability of powerful microcomputers at reasonable cost has enabled smaller-scale simulations to be built which satisfy plant personnel training needs. Caro, referring to flight simulators, has stated that " there is substantial applied research evidence that much of the training conducted in expensive simulators could be accomplished in less expensive devices "(C9). The microcomputer can be programmed to behave the same as the actual plant being simulated under control of the trainee operator. This allows the trainee to make decisions, carry out operating tasks, diagnose faults etc. so enabling him to gain experience of the actual plant's operation.

1.1 Objectives

The aims of the present study are :

(a) To develop methods of simulating chemical plant operation to achieve process personnel training objectives on microcomputers.

(b) To develop a number of generic plant unit operation training simulations to illustrate the use of the methodology.

(c) To develop a number of plant-specific operation training simulations to illustrate the use of the methodolgy.

(d) To determine the value of microcomputer-based process plant personnel training.

1.2 Layout of this Thesis

The use of computer simulation is discussed in Chapter 2. The role of the process operator and the knowledge and skill required in plant operation are examined in Chapter 3 together with traditional training methods. The use of new technologies in training and in particular computer-based-training is introduced. Chapter 4 examines the use of training simulation in the process industries. Design considerations are presented and a historical review of simulation equipment is given. The important area of fault detection and diagnosis is discussed in Chapter 5.

Chapter 6 describes the methodology employed for the computer simulation of plant operation used in this study. The selection of a suitable microcomputer system and mathematical modelling approach are discussed together with program design and development considerations. A number of examples of generic plant unit operation training simulations are presented in Chapter 7 to illustrate the use of the methodology. These examples include the operation of heat exchanger, reactor and distillation control systems. Chapters 8 and 9 present some examples of plant-specific operation training simulations. The evaluation of the value of microcomputer-based process plant personnel training is discussed in Chapter 10 and the overall conclusions of this study are presented.

Chapter 2 Simulation

2.1 Introduction

Simulation is not a new term and it can be defined as the representation of certain features of a real situation to achieve some specified objective(D7). The objective in the process industry could be for :-

(a) Design

(b) Analysis

(c) Training.

The features of the real situation are usually represented by a mathematical model and the specified objective is achieved by conducting experiments with the model. The mathematical model will consist of logical statements and/or mathematical equations. Except for a few simple systems, a computer will be needed to deal with the interplay arising from these equations and statements and to display the results of the calculations(E3). Therefore, the model is usually converted into a computer program before being used to gain experience and knowledge about the real system by experimentation.

2.2 Simulation for Design

Process simulation has been used to carry out design calculations for many years. The mathematical models used comprise steady-state material and energy balances which describe the interactions of the process variables. The objective is to determine all the values of the process parameters for a given flowsheet so that detailed equipment design can then be carried out. For example, the temperature and pressure of a flash vaporisation vessel could be determined from steady-state calculations knowing the feed conditions and the required split in the vessel. There are many computer packages available to aid the engineer in the design process such as PROCESS(P2) which runs on both large and small computers and ChemCad(B10) which runs on microcomputers.

2.3 Simulation for Analysis

Another major use of simulation in the process industries is for the analysis of the dynamics of a process. The analysis may be for the subsequent selection of a suitable control system or to assess the implications of a particular fault occuring. For example, the objective may be to determine the effect of a sudden increase in feedrate to a distillation column. Process dynamics are represented by unsteady-state material balances in the form of set of differential equations. These equations are then solved to obtain the response of the distillation column parameters over a period of time as a result of the change in feedrate.

Once again there are several computer packages which can aid the engineer in this task. These can be divided into modular and equation oriented packages. The modular approach uses subroutines that contain a differential and algebraic equation description of plant items such as a reactor, valve, distillation column etc. The modules are connected together according to the process topology and then solved in the direction of process material or control information flow. DYFLO(F4) and DYNAMIC FLOWPACK II(A8) are examples of modular dynamic simulation packages.

The equation oriented approach involves the simultaneous solution of the entire set of differential and algebraic equations which describe the problem. ACSL(H3), ISIM(C6), TUTSIM(M9) and KBCSIM(L6) are examples of equation oriented dynamic simulation packages for both mini and microcomputers. A disadvantage of this approach is that the fomulation of the set equations for a large process flowsheet cannot be done on a modular basis and therefore these packages tend to be used for small scale problems. However, some packages such as SPEEDUP(H1) include a pre-processor which allow the model to be developed on a unit operation basis. The pre-processor then arranges the equations into a simultaneous set ready for solution.

2.4 Simulation for Training

When simulation is used for training the design and development of the simulation must be governed by the objectives of the desired training. The simulation only needs to include those features of the plant which are necessary to achieve the training objectives.

Training simulation attempts to represent some or all of the operations carried out in a process plant. Gagne(G3) defines 'operations' as a set of events in which a man or men interact with machines or their environment to bring about a particular result. In this case the man is the process operator and his environment is the process plant. Therefore, a training simulation should include not only a representation of the interactions between the process variables but also a representation of the man-machine interface so that the trainee operator can interact with the simulation in much the same way as he would interact with the real plant.

The mathematical model used in a training simulation may have to be simplified in order to achieve a practical implementation without sacrificing realisim. The simulation will have to run continuously unlike simulations for design and analysis which are run batchwise. Therefore it is more important that the mathematical model exhibits a high degree of robustness rather than a high degree of accuracy.

The use of simulation in training will be discussed in greater detail in Chapter 4. The role of the process operator, the selection of training objectives and training methods will be discussed first of all in the next Chapter, Chapter 3.

Chapter 3 Process Operator Training

3.1 The Role of the Process Operator

The role of the process operator has changed dramatically over the years from one based on manual work to one consisting mainly of decision making. The operator is an integral part of the process control system. The primary function of the control system, and hence of the operator, depends on the nature of the process. In general, the main duties of the process operator are(C1):-

(a) Control
- Regulation
- Optimisation
- Changeover
- Breakdown avoidance
- Breakdown recovery

(b) Special procedures and drills

(c) Routine maintenance

(d) Recording and reporting

(e) Verbal communication.

The operator must monitor the various gauges and instruments located in the centralised control room. He must also monitor signs coming from the plant itself, such as noises, smells and vibration, and occasionally carry out special tests on the plant such as product analyses and pressure drop measurements. He must collate all this information and according to his interpretation of the indications he must adjust the controls when necessary so as to keep the product within specification and the process running as steadily as possible. He must also adjust the process conditions to give the best results according to certain criteria such as yield, quality, minimum use of power etc. In many plants, the product is changed from time to time without stopping the process, and then the operator must quickly readjust the process to the new specification so as to waste as little raw material as possible in a sub-standard product.

An increasingly important duty for the operator is to monitor the process for the early signs of faults and disturbances so that he can take preventive action. An acute operator may save large amounts of material and money by this method alone. If a failure should occur, the operator must regain normal running as soon as possible, and minimise the loss of material and risk of serious damage.

The operator must be able to carry out the set sequences of manipulation which are required when controlling a batch process, in starting up or shutting down a continuous process or in particular emergencies. These often have to be carried out rapidly and can include complicated manual operations with control activities.

The operator may be required to carry out routine maintenance such as oiling pumps and cleaning inside vessels when they become clogged.

He is responsible for recording and reporting the readings of the important indicators and gauges, control settings, and the results of any special measurements at regular intervals. He should also record the details of any fault, disturbance or changed conditions as they occur. In addition the operator should pass on information to their colleagues and management by word of mouth. For example, a control room operator will have to relay details of which manual valves to open to a field operator during plant start-up. Effective communication is important to co-ordinate the operation of the various sections of a large process plant.

3.2 Skills Required by the Process Operator

The process operator needs to know a great deal about the plant. In general, he needs training in the following areas :-

(a) Plant knowledge
   - Process flow diagram
   - Plant equipment
   - Control system and instrumentation

(b) Operating goals and constraints

(c) Operating procedures

(d) Fault administration

- Alarm monitoring
- Fault diagnosis
- Malfunction detection

(e) Emergency procedures

(f) Plant administration.

He needs to understand the process flow diagram, the unit operations of the process and the control system. The operator requires knowledge of the plant equipment and the instrumentation. In particular he needs to identify items and be able to carry out manipulations for which he is responsible. In addition, a basic understanding of the goals and constraints with which the plant management operates and the possible changes of priorities which may be necessary. He has to become familiar with numerous operating procedures such as startup, shutdown, batch operation and all other sequential routines. The operator needs to learn to administer faults and in particular interpret the alarm system, to diagnose faults and to detect incipient malfunctions. This is a particularly important task and therefore it is discussed in greater detail in Chapter 5. The operator must be throughly familiar with the emergency procedures. He must have a full grasp of the Permit-to-work system and training in fire fighting procedures(L1).

The main skills required by the process operator are those connected with the control task. The control task may vary widely in difficulty. At one end of the scale is the simple task of keeping a single variable at a desired value by means of direct control such as maintaining a flow by opening and closing a control valve. At the other end, an operator may have to maintain a combination of qualities in the product by a complex balance of conflicting requirements. It is particularly difficult to control processes where(C1) :-

(a) several display and control variables depend on one another,

(b) the process has a long 'time constant',

(c) important variables have to be estimated by the operator rather than measured by instrument,

(d) the readings of instruments at widely separated points have to be collated,

(e) the operator gets imperfect knowledge of the results of his performance or where the knowledge arrives late,

(f) the basic process is either difficult to visualise, for example chemical reactions, or contradicts 'commonsense' assumptions, or is too complicated to be held in mind at one time.

Crossman(C1) summarises the components of process control skill required by the operator as :-

(a) Sensing

(b) Perceiving

(c) Prediction

(d) Controlling

(e) Decision making.

The senses enable the operator to detect incoming signals. These can be formal such as instrument readings or informal such as noises, smells and appearance. These inputs are then interpreted by the mechanisms of perception. Signals from many sources can be combined, present inputs are compared with previous ones, irrelevant parts of the signal are filtered out and a total picture is built up to deduce the meaning and significance of the total incoming information. Much of the skill in the control task is associated with these perceptual judgments(E1).

The operator must then predict future states of the system based on the basis of the present inputs and his knowledge of the behavioural characteristics of the process. The operator must possess a full understanding of the effects of the variables under his control, particularly with regard to how they interact with one another. He must then select the control action which is most likely to achieve the desired result in the circumstances.

Crossman(C1) suggested that in making control decisions, the operator uses any of the following 'tools' :-

(a) Rules of thumb

(b) Mental model

(c) Intuition

(d) Logical approach.

The operator may follow a fairly simple algorithm based on past experience. Shepherd et al(S1) have shown that the use of rules of thumb can increase an operator's diagnostic ability. The operator may use a mental model of the process on which he can try out the different possible control actions in his imagination and decide on the correct course of action. Kragt and Landeweerd(K1) suggested that the operator possesses two types of mental model :-

(a) A 'routine' model

(b) A 'non-routine' model.

The operator appears to use the 'routine' model when controlling a process after a disturbance in control quality. The operator requires only limited knowledge of control and any additional knowledge about the process could inhibit the performance of the task. The operator appears to use the 'non-routine' model in situations in which a fault occurs. A specific knowledge of the process is necessary. The formation and updating of the non-routine model takes place only by means of the experience which the operator acquires in the course of time as he interacts with the system.

Sufficient experience could take many years to obtain and therefore the development of the 'non-routine' model will be slow. However, the development could be aided by the use of training simulation(K1). The operator's experience of the process could be increased by allowing him to further investigate the plant's operation through the use of simulations.

A good operator can develop a 'feel' for a particular process, becoming intuitively aware of what is going on and what to do about it(C1). For example, experienced control room operators walking into their plant control room at the beginning of a shift will know immediately the current condition of the process from a quick scan of the control panel. The operator may also use a logical approach to plant operations and consciously deduce the meaning of events, analyse the situation, and come to a rational decision.

The knowledge and skill required by the process operator can only be obtained by experience and through training. Wuth(W1) describes process operator training as the transfer of knowledge required to control a process. With adequate training and sufficient repetition the operator can achieve a high level of competence. However as soon as a particular skill is not used or the training stops, memory begins to fade as shown in Figure 3.1. Unless refresher training is given the skill will most likely be lost altogether. The design of training courses is discussed in the next section 3.3.

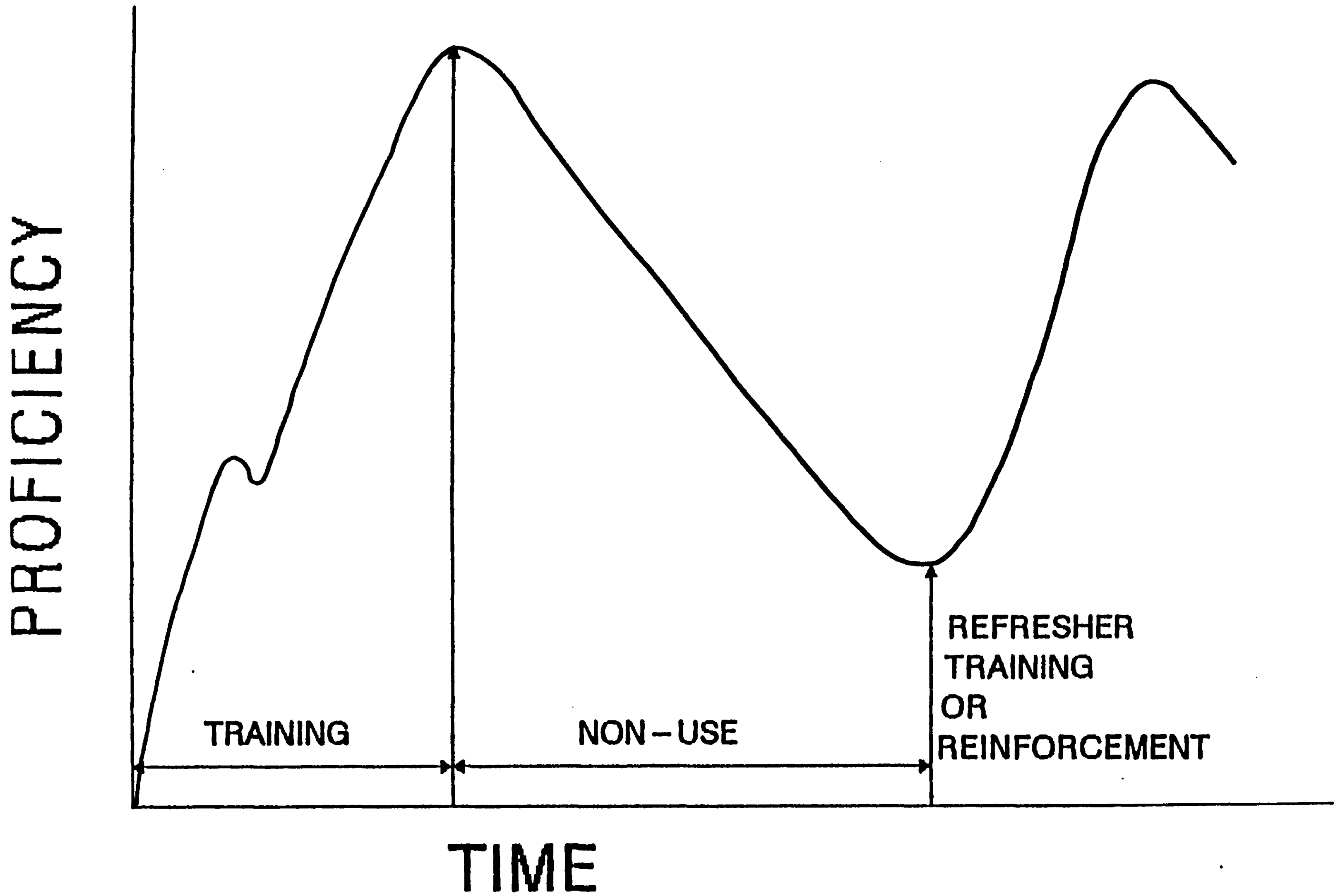


Figure 3.1 : The 'Forgetting' Curve (H2)

3.3 Training Systems Development

A systematic approach should be taken to training systems development whether it involves a whole training programme, a specific training course or just one piece of training material. Figure 3.2 shows the approach which should be taken. Once a training need has been identified by plant management a thorough analysis of the specific operator's task should be carried out to identify the actual knowledge and skill required by the operator to perform the task. Too many training courses contain elements that are of little value to the trainee in carrying out an actual task(N1). Once this has been done the training objectives can be specified and the training method selected.

Duncan(D1) describes task analysis applied to chemical plant operations. A particular task is analysed by a method of progressive redescription. The analysis begins with the most general statement of the task. The subordinate operations which are required for the task are then determined. These are then broken down into further operations until a hierarchy of subtasks which make up the main task are produced as shown in Figure 3.3. The progressive redescription into subtasks continues until the product of the probability of occurence and the cost of inadequate performance has an acceptably low value.

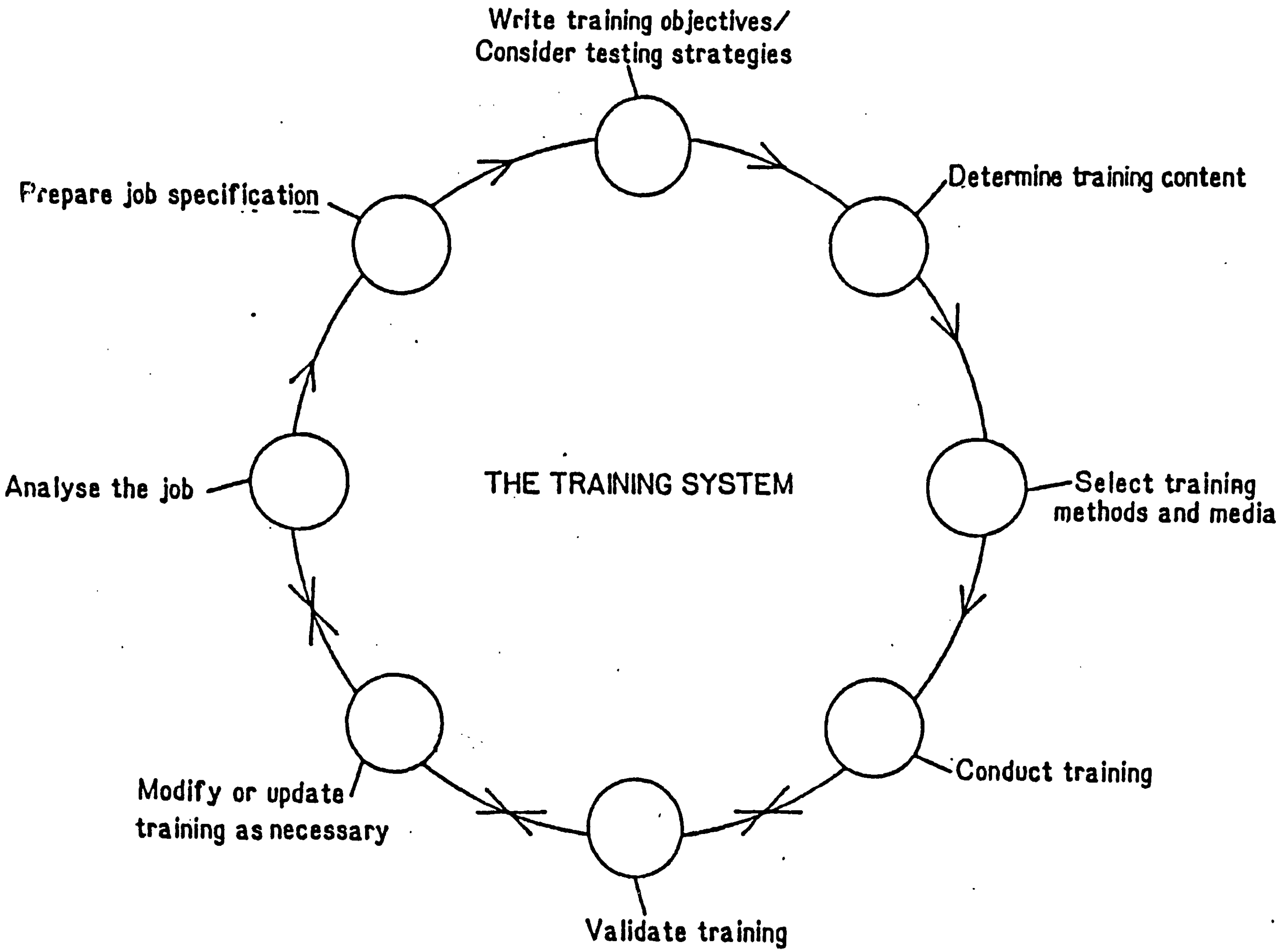
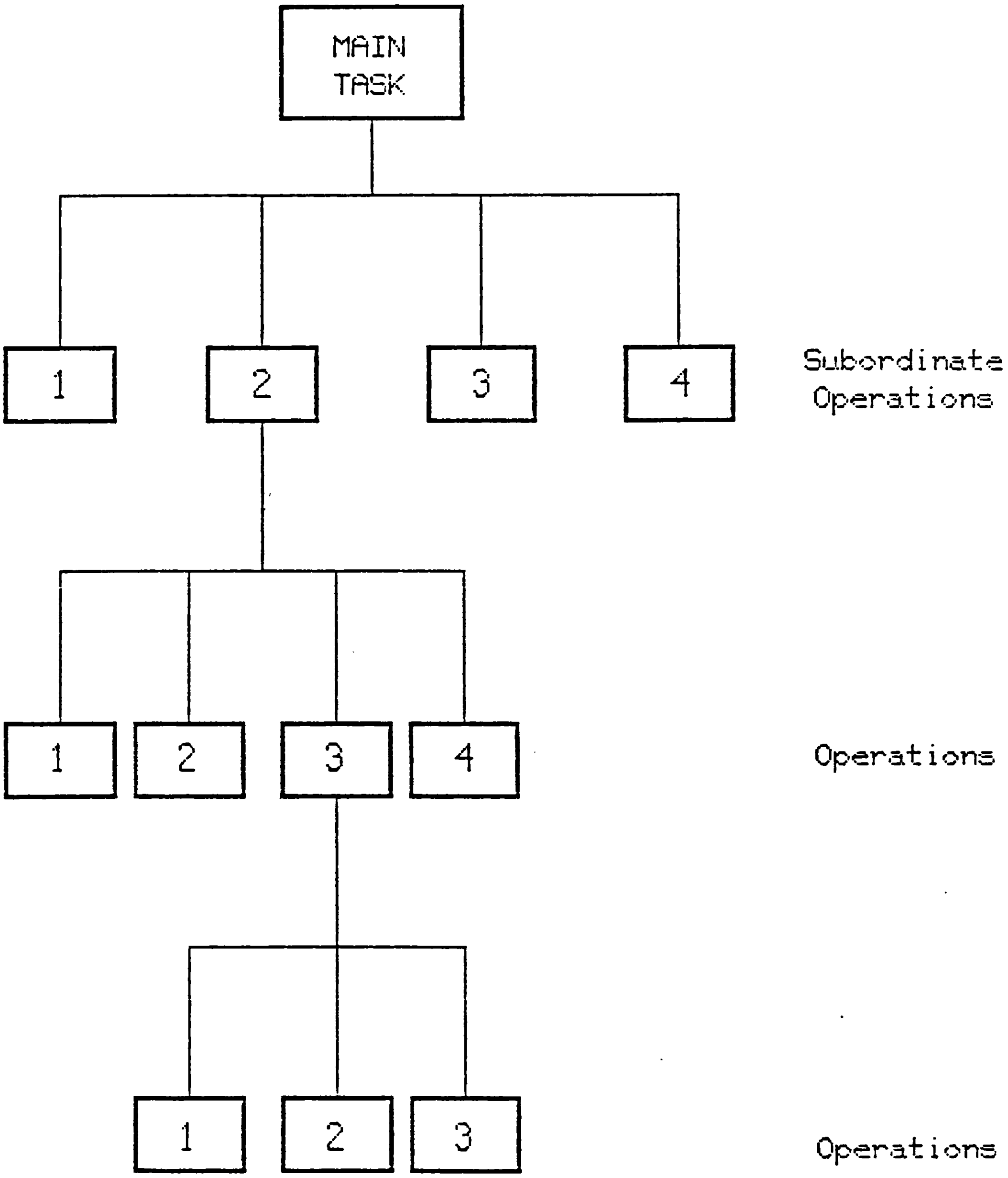


Figure 3.2 : The Systematic Approach To Training (M1)

Figure 3.3 : Task Analysis



Alternatively, the analysis ceases when the training requirement for adequate performance of the task is clear. The task analysis identifies the elements of a particular task which need to be trained and the sequence in which the training should take place.

The next stage is to define the training objectives and consider the testing strategy which will identify that the objectives have been achieved. The training objectives should state in clear terms what the trainee will be able to do at the end of the training(N1). A brief outline of the training content should then be produced based on the defined objectives and the task analysis. A suitable delivery media should then be selected.

The major aspects of selecting the delivery media are(K2) :-

(a) Identify the media attributes required to meet each instructional objective.
(b) Identify trainee characteristics which suggest or preclude particular media.
(c) Identify characteristics of the learning environment which favour or preclude particular media.
(d) Identify practical considerations which may determine which media are feasible.
(e) Identify economic or organisational factors which may determine which media are feasible.

The training objectives should determine which media is selected. For example, if an objective was to teach the difference between the various factory alarms then a medium with sound capability such as audio tape or video is required. Trainee characteristics should be taken into account. For example, if the trainees are known to be poorly motivated, then some form of interactive or highly stimulating presentation is desirable. The learning environment should also be considered. The training may have to be carried out on-the-job in a dirty environment which may preclude the use of equipment such as video players. There are numurous practical considerations such as the availability of the delivery equipment and the necessary skills needed to develop the training material. Finally, no matter how appropriate a particular medium is for the desired training it must be cost effective and affordable. Traditional training methods used in the process industry are discussed in the next section, 3.4.

Once the delivery media has been selected the production of the training material can be completed. Training should be conducted for a sufficient period to generate enough information on the effectiveness of the material and then a validation should be carried out. The training package can then be modified or updated as necessary to improve its efficiency of achieving the desired objectives.

3.4 Traditional Training Methods

Process operator training has traditionally been accomplished using one or more of the following techniques(M2) :-

(a) Classroom training

(b) Host plant training

- observation of other plant operators (hands off training)
- hands on training

(c) On-the-job training

(d) Videotaped training modules

(e) Simulator training.

Classroom training is usually a pre-requiste for all other types of training. At one time lectures were the only formal training given to operators(W1). Classroom training can be enhanced by using video-taped training modules but these cannot replace the operational situation. Host plant training could be either 'hands-on' or 'hands-off', depending on the host plants philosophy. Due to the high risk of potential damage to equipment and personnel, as well as lost production due to trainees mistakes, most host plants do not allow any 'hands-on' training on their plants(M2).

Traditionally a trainee operator would gain knowledge from an experienced operator in an on-the-job situation(W1). The trainee worked with or under the supervision of the experienced man until he felt the trainee could handle the job.

The trainee's skills were sharpened while operating the process on his own. During the supervised training period there may not have been any upsets to correct, the process probably was not shut down or started up. Training has to take second place to production priorites and the trainee's involvement may be low from a 'hands-on' and practice point of view. Consequently 'hands-on' training tends to proceed very slowly.

The quality of training received may also be poor, inconsistent, unreliable and inadequate from a probably 'untrained' expert(M1). The trainee may be trained by an operator who is already well down on the 'forgetting curve' as shown in Figure 3.1. The trainee cannot possibly learn more than his teacher so he starts out less proficient. Now he becomes the teacher of another trainee. The level of competence would drop to zero if it were not for expensive upsets which force the operators to be retrained(W1).

All these factors point to simulator training as an extremely desirable alternative. However, the use of simulation has been restricted up till now by the considerable high cost involved. The simulation package is usually included as part of major contracts only(B1). A review of process operator training simulators is given in the next Chapter 4, section 4.3.

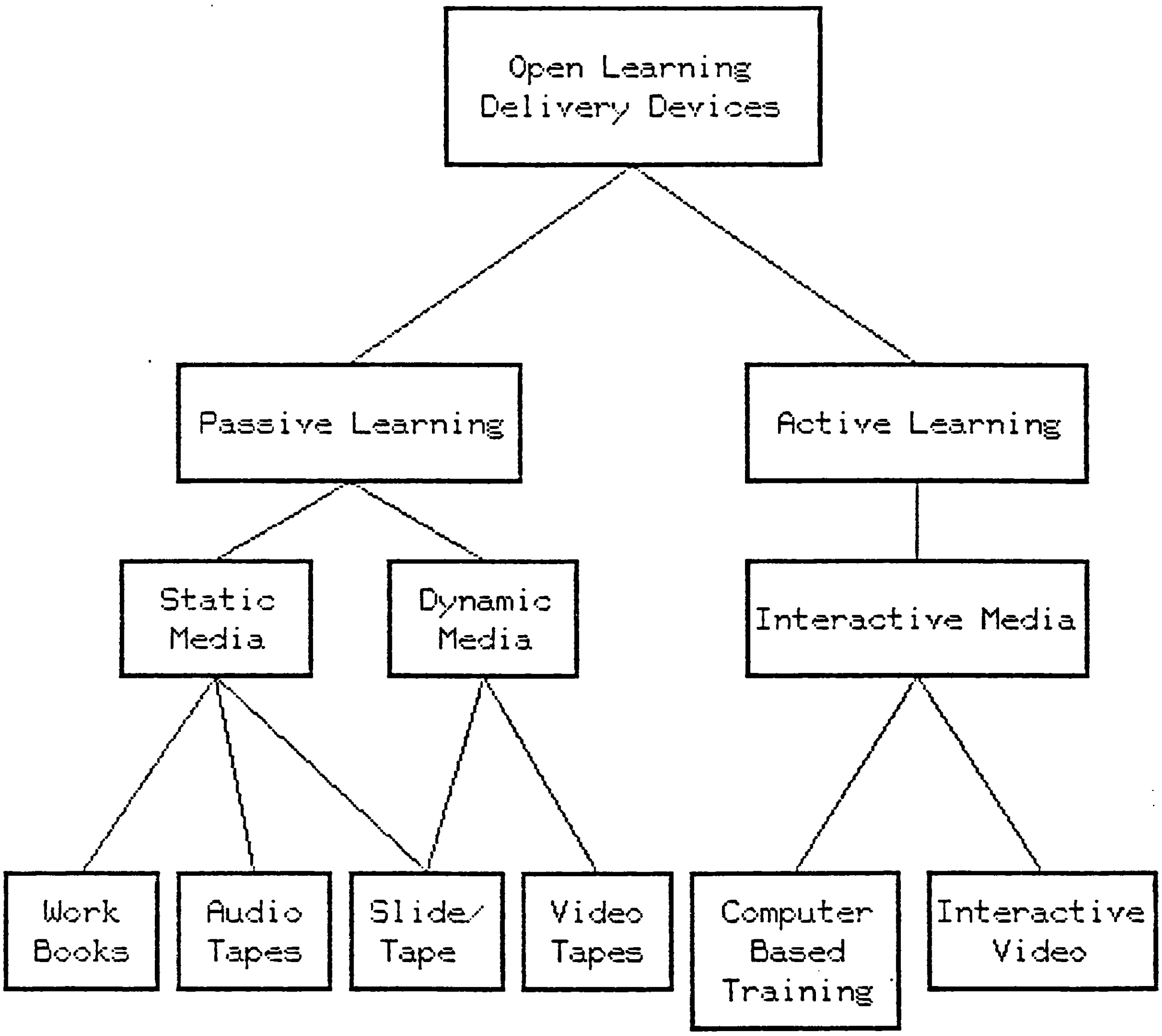
All traditional training methods require that plant operation is disrupted in some way, either by on-the-job training or by taking operators away from the plant and so causing manning problems. Training also depends on the availabilty of expert training instructors. Traditional training methods are often inappropriate or not economically viable for the small numbers of operators which staff a modern process plant(B2).

3.5 New Technologies In Training

The problem of training busy staff without disrupting plant operation has one answer in the approach known as Open Learning(F3). By this method, personnel are given individual access to prepared structured self-learning packages and allowed to progress through them at their own pace, in their own time. Training is taken to the factory floor, so that operators and technicians can have ready access to the instructional material even while carrying out their normal shift work. The training does not interrupt working schedules, it improves self-motivation on the part of the workforce, it provides a flexible and effective approach to teach new technology and techniques, and there is the possiblility of ongoing upgrading of working skills(B13).

A variety of delivery media can be used for Open Learning and these are split into those which provide a passive or active learning environment in Figure 3.4.

Figure 3.4 : Open Learning Delivery Devices



The static media include workbooks, audio tapes and slide/tape presentations. Workbooks are the simplest to use and they are particularly valuable when used in conjunction with other media. They can normally be produced using existing resources at relatively low cost. Large amounts of information can be presented and it is easy to update. Audio-tapes can be used for introductory training to a plant or factory. The portability of small personal tape recorders can be employed to provide guide-programs such as those which are sometimes used in museums.

Slide/tape devices enable slides to be displayed and sychronised with an associated audio tape. They are able to provide the visual and audio information of an instructional presentation. It can effectively replace the content of a classroom lecture or laboratory demonstration and be both a static and dynamic media depending on how it is used. However, it cannot present dynamic sequences of events and therefore video recordings are widely used for the training of procedural and interpersonal skills.

The major limitation with these audio visual media is that they can only deliver information to a trainee. They cannot actively engage the trainee in learning by providing feedback and reinforcement. Even though the trainee may spend many hours reading a workbook, listening to an audio tape or watching a slide/tape presentation, without active response and interaction there is no way to ensure learning is taking place until a practised exercise or test is carried out(K2).

The use of computers in training allows a high level of interaction to be included in training presentations. Trainees assume an active role which has been proved optimal for learning. Computer-Based-Training or CBT is a general term which covers both the topics of computer-assisted-training and computer-managed-instruction(D2). Computer-assisted-training means using the computer as an interactive training medium to display training material. Computer-managed-instruction means using the computer to direct a trainee through a course, which may, or may not, be computer based. The path the trainee follows is dependent on the results of tests and measures of performance taken during the course. CBT will be discussed in greater detail in the next section 3.6.

A further new training technology which will find increasing use is the combination of a computer with a videodisc player. The visual perspective provided by interactive videodisc presentations has a realism and fidelity not achieved with textual and graphically based systems(B4). The computer generated text and graphics are replaced or combined with any one of the 54000 visuals available on a videodisc. Therefore, for example, a trainee can see and interact with a video picture of the actual plant control panel with which he will be working. This is very useful in familiarisation training where the trainee has to learn the knobs and dials associated with a particular control system. The use of interactive video is restricted at the moment due to the high cost involved in producing the actual videodisc in the small numbers required for custom applications. As this cost comes down, interactive video will take its rightful place along side the other new technologies in training.

3.6 Computer-Based-Training(CBT)

CBT has many benefits over traditional training methods(T1). The training does not depend on the availability of expert training instructors, but is available whenever it is needed. An operator with free time during a night shift, for instance, can obtain dynamic, high quality, training. Training can be delivered directly to the trainee, thereby saving the cost of instructor or trainee travel and living expenses. Operators can be trained at their plant and be readily available when emergencies or demanding situations arise. The training is consistent and thorough. The training can be private, to allow trainees to ask and answer questions and 'teach themselves' at their own pace without embarrassment. The training can be further individualised so that trainees receive what they need and only what they need. A course can be valuable for different personnel, as each can take only the modules which are relevant to his or her own job. No other instructional medium can be as adaptable to the characteristics of the trainee. Trainee performance can be recorded to allow assessment or decide what activities should be prescribed for the trainee to do next.

Proficiency can be assured by providing practice and remedial help until the desired level of mastery is reached.

A wide range of instructional programs can be provided, giving explanation, demonstration, drill and practice, or experience as required. The computer can simulate a variety of complex operations and activities, so that trainees can observe and analyse them and practise their responses realistically. There are three main categories of CBT modules(T1) :-

(a) Drill-and-practice

(b) Tutorial

(c) Simulation

In drill-and-practice CBT the computer presents a series of examples to help the trainee develop proficiency in a specific skill. The computer provides guiding feedback to enable the particular skill to be learnt. For example, drill-and-practice CBT has been used to teach operators compressor start-up procedures(B2).

Tutorial-mode CBT is an extension of traditional book-based programmed learning. The computer presents information to the trainee via text and graphics. Animation is judiciously used to make the presentation more dynamic and effective. The computer will determine if the trainee has mastered a topic through testing. It will provide suitable feedback, possibly including remedial information and adapts to the trainee's performance when appropriate.

An example of tutorial-mode CBT is seen in the teaching of radioactive protection to nuclear power plant operators(P1).

In simulation-mode CBT the computer is programmed to behave the same as the actual plant being simulated under the control of the trainee. The trainee is able to learn by discovery. The computer's graphic capability is used to represent the plant instrumentation and to reproduce the control panel to an acceptable degree. The mathematical capability of the computer can be used to carry out the simulation calculations which model the operation of the plant and the process dynamics are displayed by means of animation. CBT simulations have been used in the nuclear power industry(T1),(J1).

CBT has been used for process operator training in the UK(B2), USA(B7) and in Italy(B8). It has been used to enhance the chemical engineering curriculum in several universities in the USA(S2),(E2). Shacham and Cutlip described its use in chemical reaction engineering(S3),(S5) and as an aid to simulation studies(S4).

The most powerful use of CBT must be in providing relatively low cost, highly interactive instructional simulations for use in process plant personnel training and in general chemical engineering education within Universities and Polytechnics. In particular, it will allow the process operator to improve his 'non-routine' mental model of the process and practise his fault diagnostic skills.

Chapter 4 Training Simulation

4.1 Introduction

The most familiar example of the use of simulation in training is the use of flight simulators for pilot training. Simulators are used among other reasons to reduce cost and eliminate the inherent dangers of training in the real life situation(M1). Simulators possessing suitable characteristics for process training evolved very slowly from the aerospace industry experience during the 1960's. The process industry did not need new methods of training because(D8) :-

(a) Few new-technology plants were being built.
(b) Energy supply and environmental standards were not key issues.
(c) Very little recruitment of new operators.
(d) Time allowed most training to be done on-the-job.

The importance of simulator based process operations training grew during the 1970's for several reasons(C3) :-

(a) New and complex process technology required broader and more comprehensive training.
(b) Industry growth dictated more efficient training to accomodate increasing numbers of trainees.
(c) Remote plant sites required adaptable and mobile training devices.

(d) Plants in developing countries had special training requirements for the available labour force.

(e) Highly integrated processes and rising energy costs placed a premium on intelligent and efficient operation.

There are three parts to a training simulation(M1) :-

(a) The mathematical model

(b) The simulator or necessary equipment

(c) The training application.

The design of the mathematical model and its implementation will be considered in the next section 4.2. The type of equipment utilised will be discussed in section 4.3 and the applications of training simulation in the process industry will be considered in section 4.4.

4.2 Design Procedure and Considerations

The design of an operator training simulation should be governed by three factors(U1) :-

(a) The objectives of the training programme

(b) The population to be trained

(c) The design of the plant.

The selection of training programme objectives was discussed in Chapter 3, section 3.3. For example Uttamsingh and Shinohara(U1) describe the development of a simulator based training programme for the Alexandria Petroleum Company(APC) in Egypt. A new lube oil plant which was under construction was to use process technology and digital control instrumentation which was unfamiliar to the Egyptians. A training programme was required to train 39 inexperienced trainees all they needed know in four months to serve as operators on the new plant.

The population to be trained consisted of trainees of varying levels of operating experience from 12 years on similar plants to recent engineering graduates. Training objectives were defined and a training programme utilising a simulator was developed whilst considering the needs of the training population. All trainees were unfamiliar with digital instrumentation but using the simulator they became familiar with a digital system, and increased their skills until they could control the process just as well, if not better than with analog instruments.

The plant design affects the development of the mathematical model and the equipment on which it is implemented. France(F1) describes how the training simulation should be derived. It involves four stages :-

(a) Preparation of functional specification

(b) Collection and collation of plant data

(c) Model development

(d) Model loading, debugging and acceptance testing.

The preparation of the functional specification involves identifying the plant or section thereof to be simulated and the essential elements to be included. The model must be large enough to include everything necessary to develop a satisfactory training programme and yet be constrained by practicality. For example, start-up and shutdown lines, bypass lines and the utility systems need only be included if they are going to be part of the training exercise. Having defined the area of the plant to be simulated, it is necessary to define those pieces of equipment, piping, valves etc. which will be included in the simulation. The product of these two steps is usually a P & I diagram of the plant as it will be simulated.

The next step is to identify the process variables to be interfaced with the control system. It is generally not practical to include in the simulation all measurements that would exist in the actual plant, since this would mean a simulated control system equal in size to the control room instrumentation. The number of variables must be consistent with the training objectives of the model. The selection of malfunctions, if they are to be included, is very important. They should represent where possible each of the different types of process and equipment upsets that are likely to occur on the real plant.

The specification should also identify any field operator functions which are required such as the operation of valves and pumps that are not accessible to the control room operator but must be manipulated under his direction by the field operator.

At this point, the equipment on which the simulation is to be implemented should be selected. The training objectives have been derived from a task analysis so that at the end of the training programme certain operational tasks are better performed. These tasks should be taken into account when selecting the equipment to be used.

For example, suppose oil rig drillers are being trained in the procedures associated with the drilling operation. There is no need for the simulator to include the actual brake handle, dog clutch and foot throttle used to control the drill bit(R4). However, if the objective of the training is to teach the motor skills required in controlling the drill bit then the simulation of the actual controls becomes very important. Similarly, if the objective is to train conceptual tasks such as diagnosing faults from a control panel then only a representation of the control panel instrumentation and readings is required rather than a replica of the actual panel(D7). In general, studies have shown that fairly radical departures from physical similarity can produce high degrees of skill and knowledge transfer from a simulated to an actual task(G3).

The computer equipment which has been utilised for process operator training simulators are described in section 4.3.

The next stage is the collection and collation of the plant data. This data should include a basis for process design, heat and material balances, thermodynamic properties of all fluids, equipment specification and configuration including such details as control valves, pump characteristics and operating procedures. If the training programme is to cover start-up and shutdown procedures then the data must also cover all operating conditions from cold start to maximum throughput.

A mathematical model can then be developed to represent the plant. Training simulation involves the simulation of process plant interactions and dynamics. Most applications of dynamic simulation involve analysis of the dynamic behaviour of a model representing the equipment or process of interest. Therefore, it is important for the model to be a detailed mathematical representation so that the responses of the model to disturbance can be studied to predict the behaviour of the real system. The converse is true with training simulation models since the responses of the model to disturbance are known beforehand. This prior knowledge of model responses enables the mathematical model used to be simplified. The models are simplified in order to achieve practical implementation without sacrificing realism. In addition, 'exactness' or sophistication in modelling may not be practical if it requires data which are not readily available or does not enhance the simulation results. To be cost effective, most training simulator responses to disturbance are correct in direction only and are not exact in magnitude when compared to the actual plant(C4).

Mathematical equations which may be algebraic, boolean and/or differential are written to represent the theoretically expected plant behaviour. Coefficients within the equations are then 'tuned' so that the equations represent the particular plant's behaviour. Mathematical modelling for use in training simulations will be discussed in detail in Chapter 6, section 6.4.

The model is then loaded into the computer and debugged. Finally acceptance testing is carried out which involves having the programme evaluated by experienced plant personnel and validating the simulation against known process data. If a simulator is to be of real value as a training aid it must be accepted by plant personnel as being a valid substitute for the real plant. This means that the operators must be able to identify operating situations which arise, or which are created on the simulator with the similar situation on the real plant, and can then manage the situation as they would do on the plant(D4). The design of interactive microcomputer-based training simulations which are the subject of this work is described later in Chapter 6.

4.3 Training Simulator Equipment

4.3.1 Introduction

Training simulators have been used in industry for many years and they vary greatly in complexity. Training simulator equipment consists of two components:-

(a) The Operator interface,

(b) The machine or computer which simulates the plant's response.

Clymer et al(C3) define simulator types based on how much of the operator's task is represented and how well the simulator reproduces his working environment :-

(a) A 'replica' simulator contains a complete and exact duplicate of the man-machine interface and a realistic rendering of the multi-sensory environment of the system simulated.

(b) A 'generic' simulator is a representation of a class of systems but is not a replica of any one.

(c) An 'eclectric' simulator includes deliberately a mixture of features, such as several different manufacturers instruments to provide a broader experience to the trainee.

(d) A 'full task'(or 'full mission', 'full scope' or 'full scale') simulator deals with the entire task of the operator in his command of the system.

(e) A 'part task' simulator is concerned with only part of the operator's task or mission, or else with only part of the system that he operates, or part of each.

(f) A 'basic principles' simulator is a 'generic' and/or 'part task' simulator that omits many details in the interest of economy and simplicity. It is capable of demonstrating all of the important gross behaviour of the system.

Training simulators can also be classified according to the equipment used to simulate the plant's response. They can be mechanical, or use analogue or digital computers, or they can 'piggyback' on the existing process control computer or more recently use microcomputers.

'Replica','full-task' simulators are extremely expensive to develop and consequently their use has been confined predominantly to the aircraft and nuclear power industries. A typical 'replica','full-task' nuclear power plant simulator features an exact replica of the control room environment which an operator would find in a real power station as shown in Figure 4.1. A dupilcate of the actual plant control room instrumentation is used which provides proper indications in response to operator control actions. A seperate instructor station is provided so that the instructor can set up and monitor the training exercises. Using the station he can introduce malfunctions into the mathematical model and establish the quality of the operators response.

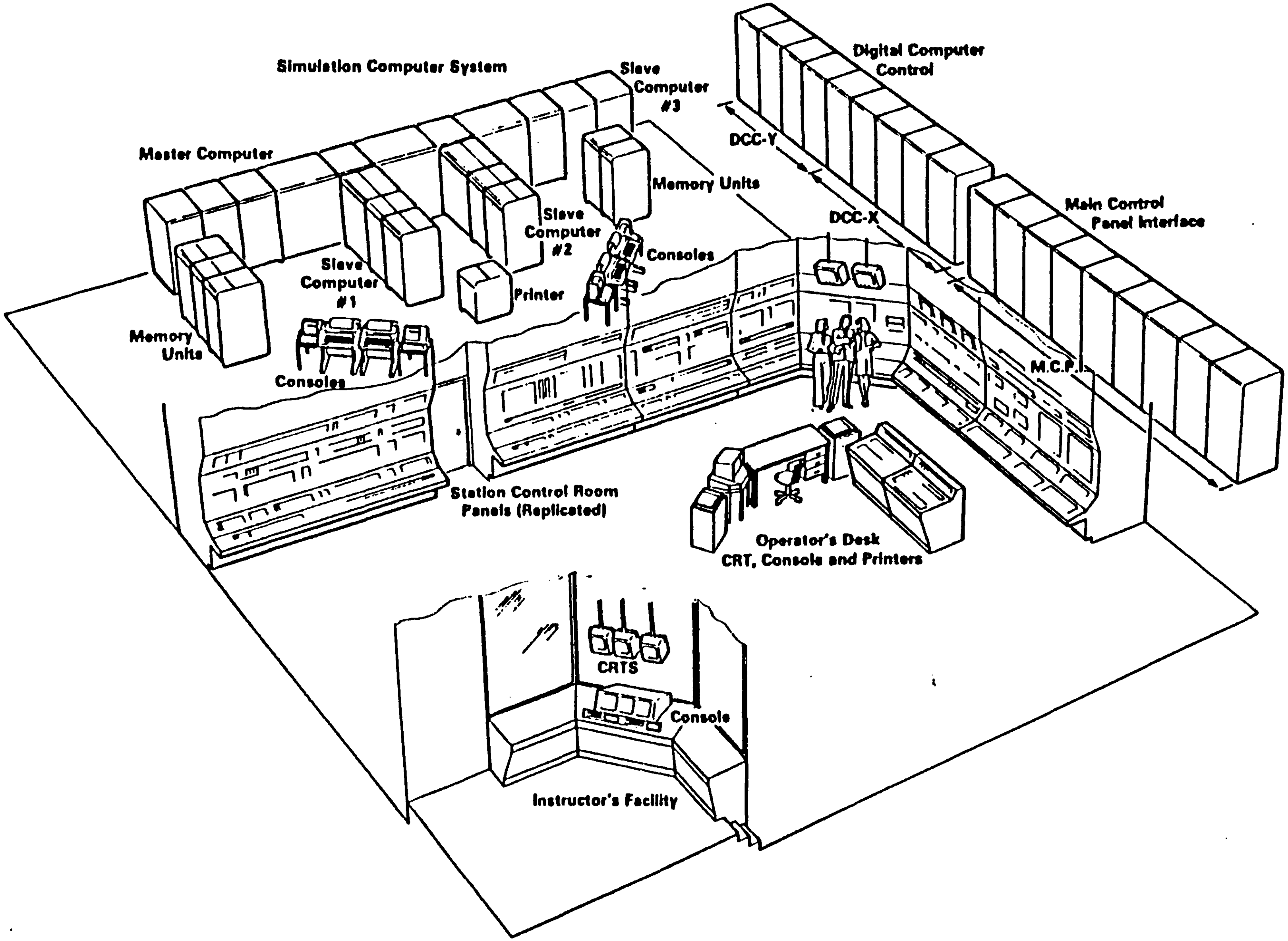


Figure 4.1 : Nuclear Power Plant Simulator (C5)

Steven(S9) reports that the realism of the simulated control room would not be complete without some audio/visual stimuli which recreate the atmosphere of the real control room. He describes a simulator where audio/visual effects such as turbine generator, safety valve and control room instrument noise is generated together with dimming of the control room lamps.

The simulator is driven by a substantial computer system which carries out the extensive calculations which are required to represent the behaviour of the plant in real time. Table 4.1 gives the hardware and software used in the Hunterston B Advanced Gas Cooled Reactor simulator. 10 MBytes of computer memory and over 12000 equations are required.

Table 4.1 Hunterston B Advanced Gas Cooled Reactor Simulator Hardware and Software Specification(W2)

Number of microprocessors	52
Total memory capacity	10 MBytes
Total hard disk capacity	56 MBytes
Number of colour graphic displays	6
Number of high speed printer/plotters	4
Number of digital I/O channels	8000
Number of analogue I/O channels	1000
Number of differential equations	3500
Number of algebraic equations	4000
Number of Boolean equations	5000

In addition, the computer has to perform the non-simulation tasks associated with the instructor's console and the generation of the audio/visual effects. Steven(S9) describes the various instructor aid programs that are available on the simulator manufactered by Electronic Associates Inc. in the USA. These programs range from initial condition setting and variable monitoring to the introduction of random malfunctions and 'crywolf' alarms which are alarms that appear randomly on the annunciator panel or alarm typewriter.

The extreme cost of the 'replica','full-task' simulator can only be justified for severe training applications such as those already mentioned where the slightest error could have dire consequences. The process industries use of training simulators has developed on a much smaller scale. Table 4.2 gives a list of a number of training simulators used in the process industry. They are classified according to the previously defined criteria of equipment used and fidelity of the implementation.

4.3.2 'Mechanical' Simulators

The early training simulators used in the process industry in the late 1960's were mechanically driven control panels. Roberts(R5) described the Simtran Process Panel Simulator(PPS-1).

Table 4.2 Process Operator Training Simulators

Ref	Author(s)	Type	Classification	Application(s)
(B6)	Bakhai, R. Marr, G.R.	Analogue /Digital	Part Task/Generic	Unit Operations
(R3)	Rubin, A.I. Pathe, D.C.			
(K5)	Kopy, W. Liotta, F.J.			
(B11)	Bainbridge, L. Beishon, J. Hemming, J.H. Splaine, M.	Analogue	Part Task/Generic	Furnace
(B7)	Beech, G.	Micro	Part Task/Mimic	Plastic Film Manufacture
(B9)	Berthoumieux, J. LaCava, A.I.	Digital	Part Task/Generic	Heat Exchanger
(B5)	Bond, A.	Analogue	Part Task/Generic	Unit Operations
(C2)	Collacott, E.A.	Mech	Part Task/Generic	Unit Operations
(D4)	Davies, J.	Analogue	Full Task/Generic	Substitute Natural
(D5)	Davies, J.			Gas Plant
(D3)	Doering, R.D. Bauer, C.S. Silkensen, G.R.	Micro	Part Task/Mimic	Waste Water Treatment
(D6)	Doig, R.M.M.	Digital	Part Task/Replica	Batch Processes
(E4)	E.E.S.M. Ltd	Digital	Part Task/Generic	Unit Operations
(F1)	France, D.W.	Digital	Part Task/Replica	Furfural Unit
(F2)	Fertik, H.A.	Digital	Part Task/Control	Breakpoint Chlorination Activated Sludge

Table 4.2 cont. Process Operator Training Simulators

Ref	Author(s)	Type	Classification	Application(s)
(G1)	Gauthier,J.P.	Digital	Part Task/Generic	Petrochemical
	Nougaret,M.			Unit Operations
	Bornard,G.			
(G2)	Gray,M.J.	Digital	Part Task/Mimic	Batch Control System
(H1)	Herman,D.J.	Digital	Part Task/Control	Furnace
	Sullivan,G.R.			
	Thomas,S.			
(I1)	I.C.I.	Digital	Full Task/Replica	AMV Ammonia Plant
(J2)	de Jong,P.J,	Digital	Part Task/Control	Naphtha Cracker
	de Wijn,W.J		Part Task/Replica	Urea Stripping
(K3)	Kalani,G.	Digital	Part Task/Control	Oil Production Unit
(K4)	King,M.	Micro	Part Task/Generic	Control Systems
(K6)	Kobe Steel Ltd	Digital	Part Task/Generic	Cement Plant
(L2)	Lieber,R.E.	Analogue	Part Task/Generic	Refinery Start-Up
	Herndon,T.R.			Operations
(L3)	Lummus Co.Ltd.	Digital	Part Task/Generic	Utility Boiler
(L5)	Lummus Co.Ltd.	Digital	Part Task/Replica	Lube Oil Refinery
(M5)	Mostafa,E.S.			Unit Operations
	Bassyoni,A.			
(U1)	Uttamsingh,R.			
	Shinohara,T.			
(M2)	Madhavan,S.	Micro	Part Task/Generic	Ammonia Plant

Table 4.2 cont.   Process Operator Training Simulators

Ref	Author(s)	Type	Classification	Application(s)
(M6)	Marshall, E.C. Brooke, J.B.	Digital	Part Task/Generic	Simple Unit Operations
(M3)	Murtha, S.A. Glaser, D.C. Amin, C.R.	Micro	Part Task/Replica	Depentaniser Column
(M4)	Murtha, S.A.	Micro	Part Task/Generic	Unit Operations
(A1)	Atlantic Simulation Inc.			Instrumentation
(N2)	Nakajima, K.	Digital	Part Task/Replica	Ammonia Plant
(R1)	Records, L.R. Romaguera, D. Sonnier, C.	Micro	Part Task/Generic	Oil Rig Drilling
(R4)	Rediffusion	Digital	Full Task/Generic	Oil Rig Drilling
	Simulation	Micro	Part Task/Mimic	Hydrostatic Sterilizer
(M1)	Ltd.	Digital	Full Task/Replica	North Sea Oil And Gas Production Platform
(R10)	Rice, V.L.	Micro	Part Task/Generic	Distillation Columns
(R2)	Roberts, D.H. Dobie, F.	Analogue	Part Task/Generic	Unit Operations
(R5)	Roberts, L.	Mech	Part Task/Generic	Unit Operations
(R6)	Roberts, L.	Analogue	Part Task/Generic	Unit Operations
(S7)	Singer Link Simulation Division.	Digital	Part Task/Replica	Natural Gas Plant Polymer Plant
(S6)	Shinohara, T. Ricci, L.	Digital	Part Task/Replica	Naphtha Cracker Ethane Cracker
(T4)	TQC Ltd	Digital	Part Task/Generic	Unit Operations

This consists of a mock-up of a control room panel, with a series of full size models of analogue process instruments, together with a magnetic process flow diagram display board which gives the layout of the process being simulated. The panel contains 27 process control instruments, four ribbon type indicators, a multipoint temperature indicator, a bank of six alarms linked to a klaxon and four sets of on/off buttons which are linked to indicating lights on the display board to represent power driven equipment such as pumps and compressors.

An instructor control console attached to the panel by a multicore cable allows the instructor to adjust the process variables in relation to the trainee's actual operation of the panel mounted instruments. All plant responses to operator actions, or to process faults and upsets, have to be generated by the instructor. The instructor has to act as the model of the plant. A great deal of concentration is required from the instructor to avoid making mistakes such as allowing an indicated flow through a line in which a block valve is still shut (one which the instructor has missed!). Roberts(R5) pointed out that if the simulation is particularly complicated then the instructor needs more than the usual complement of hands to be able to operate all the chart pen recorders and their responses to the trainee's actions!

4.3.3 'Analog' Simulators

In the early 1970's automatic process training simulators became available with an analog computer being used to provide the model of the process. Clymer et al(C3) and Bakhai and Marr(B6) described the Model 1501 Simulator Trainer manufactured by Autodynamics Inc. in the USA. The simulator is shown in Figure 4.2. It consists of five elements, the process 'graphic', the trainee's control panel, the computer section, the program drawer and the instructor panel. The front panel is arranged like a section of a control panel. At the top is the process graphic showing the plant flowsheet and below this there are 15 three-mode controllers together with alarms and indicators. The individual user selects the brand and model of instruments which are most appropriate and the panel layout which best serves his application. A printed magnetic tag is located below or beside each hardware element. The analog computer is housed beneath the panel. At the bottom right 'plug-in programs' can be loaded into a drawer. These programs are analog simulations of particular process operations and they can be combined together to form a model of the plant.

The upper part of the right hand side panel contains the instructor portion of the console. This enables the instructor to insert and remove faults, switch off, switch on, suspend the simulation and to insert initial conditions or change parameters whilst the simulation is running.

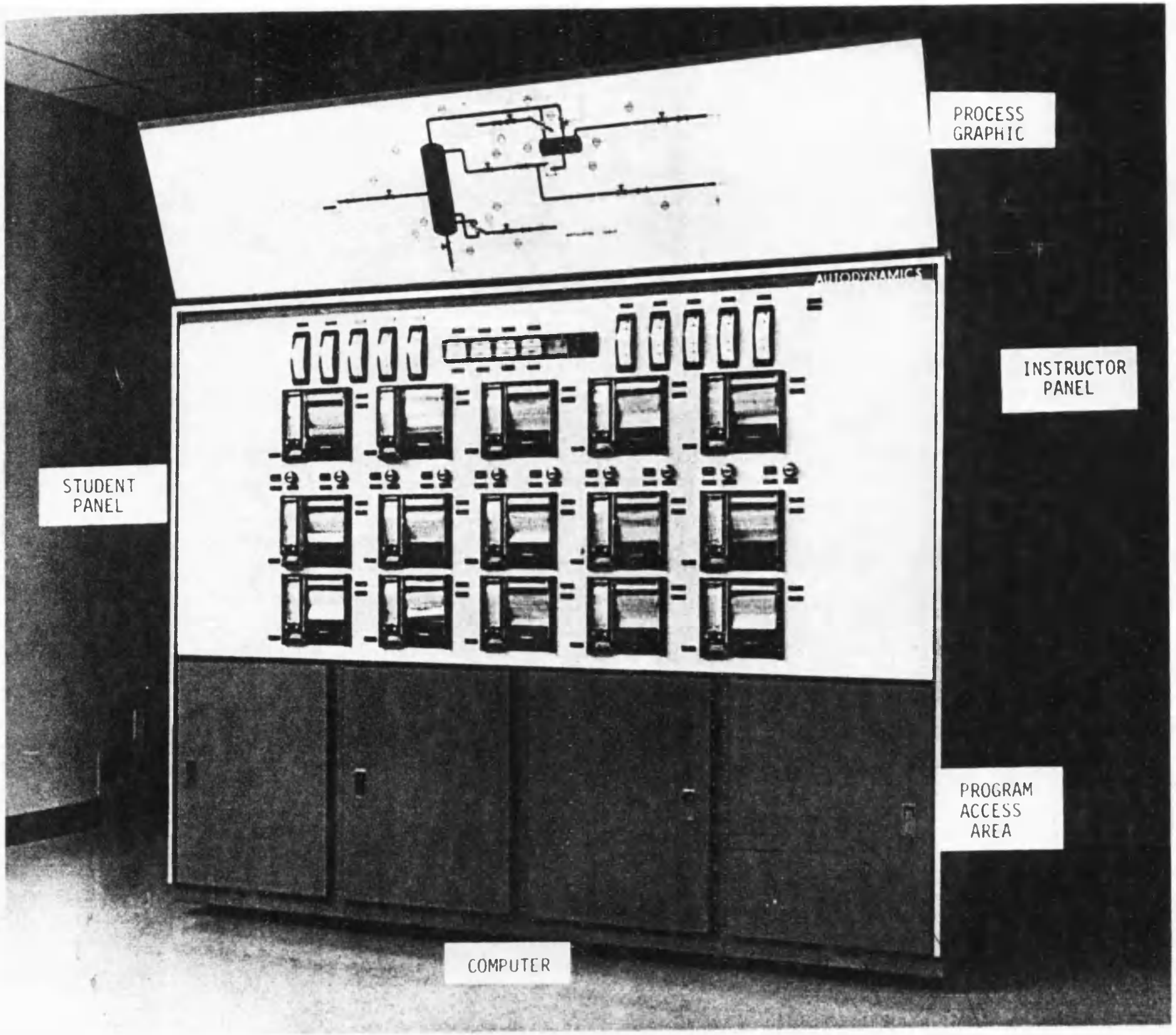


Figure 4.2 : Process Operator Trainer (C3)

The simulator can be used to represent different sections of a plant at different times by changing the process graphics, the 'plug-in' computer program and the magnetic tags on the trainee and instructor panels. It was widely used for 'part-task' training and it attempted to make the man-machine interface as close as possible to a real control room whilst retaining flexibility and mobility.

4.3.4 'Digital' Simulators

In the present day the analog computer has been replaced by the digital computer. The most recent major development in process operator training simulator hardware is the development of the PROGRES Operator Training Simulator by CE Simcon, formerly part of CE Lummus(F1),(L5). The PROGRES Operator Training Simulator consists of a digital simulation computer which drives both an instructor and a trainee station. The trainee station is a realistic replica of the controls and displays, either analogue or digital, which the trainee would use on the actual plant. The trainee is able to learn how to start-up and shut down the plant and how to deal with disturbances, emergencies and requests for changes in operating conditions. Radio communications, recording and logging devices, telephone and other distractions are included and the instructor can generate the sort of inconvenient interruptions with which the trainee operator will have to live.

The instructor station can be either a hand-held keypad or a CRT display with full keyboard linked directly to the simulation computer. Through it, the instructor may specify initial conditions which could be either a custom condition specific to a particular plant, normal operating conditions or an intermediate step in the start-up routine. In addition, the instructor can insert disturbances into the process to simulate a variety of equipment malfunctions and fault conditions. He may also freeze, restart or re-run the simulation as well as manipulate various remote functions to simulate the action of a field operator.

The simulation routines are written in a block structured simulation language called GEPURS(GEneral PURpose Realtime Software) developed specifically for PROGRES by CE Lummus. The block structured technique is described by Shinohara and Cowley(S10). Algorithms for mathematical functions, transfer functions and process equipment were developed and structured as individual blocks within a special block executive. The algorithms were at first programmed in assembly language to speed up the system execution. However, the block executive can also call routines written in FORTRAN so that unusual calculations not included in the block library can be performed.

The PROGRES simulator is available in three levels of sophistication. The full simulator uses a custom plant model which is specific to a given plant. The plant's own operating procedures and plant data are used in the model which can be as small as a single reactor for 'part task' training or as large as an entire refinery for 'full task' training. The simulator can also be used for control system analysis and as a partial design check on the engineering of the plant(F1). A PROGRES simulator of this type has been used by the Alexandria Petroleum Company in Egypt to train inexperienced operators for a new lubricating oil refinery(L4),(M5),(U1).

The second level is the 'generic', 'part task' simulator which uses a generic, 'standard plant model'. This duplicates a typical but not specific plant. It exposes the trainee to plantwide operating procedures. It shows the operation and interaction of specific pieces of equipment which enable the trainee to see the plantwide reaction to changing just one process parameter. A 'generic' model of a drum-type utility boiler is described in (L3).

The third and simplest level is the 'basic principles' simulator which uses a 'standard unit operation' model. These are confined to a small section of plant or a major piece of equipment. These models are not specific to any particular plant but are used to teach the trainee the concept of operations, for example, the operation of a fired heater or a typical distillation column.

Most modern plant's use digital computers to monitor and control the process. There are benefits to be gained if the process control computer is also used to implement simulations for training(F2). For example, the operators and instrument technicians could interact with plant models through the actual control room interface. This allows operator training to be carried out without having to invest in highly expensive training simulator hardware. The plant simulation models can be coded in the language used to program control algorithms if the language has a provision to represent system dynamics and disturbances. Since the process control language is designed for interactive execution, the programming may be simplified when compared to a simulation language since many of the same software elements used for control can be employed in building up the plant model. Fertik(F2) has described the technique applied to breakpoint chlorination and activated sludge processes in the water industry.

4.3.5 'Microcomputer' Simulators

The current rapid advance of digital computer technology in the 1980's has accelerated the possible use of microcomputer based systems as plant operation simulators. Madhavan(M2) described a microcomputer based simulator for the Kellogg Ammonia Plant. It was developed with the cooperation of Atlantic Simulation Inc. and uses a microcomputer, two CRT displays, two keyboards and a printer. The simulator can easily be accomodated on a desk top. It achieves much of its compactness and cost effectiveness by combining the control system and process aspects of the simulator into one computer.

The microcomputer handles the process simulation, instructor control functions and a filing system for simulation data. The two colour graphic CRT's are used to display process flowsheets and to mimic the displays and interactions associated with the operator interface. The trainee interacts with the control system via one of the keyboards and a CRT. He can change controller setpoints, outputs, control modes, controller tuning parameters and alarm limits.

The training exercise is controlled with software accessed through the second console by the instructor. Process conditions and equipment failures can be activated using menu driven displays. In addition, all the switches that are available to the trainee may also be controlled by the instructor. Any desired change can take place immediately or they can be placed in a queue to be activated at specific times. The instructor may freeze the simulation to discuss important features with the trainee and select start-up conditions for training execises. Each simulation program has a data base which stores control system information, initial conditions, graphic images and historical data for trend displays.

The UCSD Pascal language system is used to program the simulation although time critical procedures such as input/output functions are coded in assembly language. The dynamic behaviour of the processing equipment is modelled with a set of differential equations. The equations are solved numerically to yield the process parameters. The simulation is based on the ammonia process flowsheet, the material and energy balance and the training objectives. It can model the normal operation, start-up and shutdown procedures and a number of abnormal and emergency conditions.

Murtha(M4) claims that microcomputer based training simulators are portable and relatively inexpensive and they "open the door for widespread use of simulation training in the process industries". They could be further enhanced by incorporating them into CBT programmes as mentioned in Chapter 3, section 3.6 and this will be described in more detail in later chapters as the main subject of this work.

4.4 Uses in the Process Industry

Training simulators can be utilised for variety of training purposes(C3),(M7) :-

(a) Familiarisation

(b) Skill development

(c) Knowledge of plant

(d) Decision making

(e) Fault diagnosis

(f) Team working.

The most popular use for training simulators in the process industry has been in familiarising operators with processes and plant. Operators who are new to process work or who are changing from one plant to another need to be totally familiar with the plant flowsheets and be able to relate the symbols to specific control panel hardware. Simulation increases the flexibility of process operators on different plants and processes.

In addition, plant modifications are made from time to time and frequently these modifications result in changes in the operating procedures and control room instrumentation. In some instances, learning these modified procedures can present a significant problem since the differences between the new procedures and the old might be slight. In times of stress an operator must be able to recall immediately the most recent procedures and must not by mistake find himself reverting to outmoded procedures which may increase danger to himself and to the plant(M7). Simulation enables the procedures to be practised regularly and so reduce the chance of error under stress.

Skill development includes both basic and advanced skills, such as reading of instruments and meters, setting of controllers etc. to more complex skills such as avoiding compressor surge and start-up and shutdown of particular units. In addition, operators can learn to optimise the process variables and so achieve more economic operation.

Knowledge of plant is desirable in all operating personnel to give them an appreciation of the interactive and interlocking nature of the plant's units. The operators should appreciate, understand and even be able to predict the effect of an action taken at one unit on the rest of the plant. Simulation training is one of the most efficient ways of gaining this knowledge(C3).

Proper decision-making can save a unit, a plant, and human lives, knowing how to recognise dangerous situations and taking the right course of action are vital aspects of this skill. Plant operators should also be skilled in fault diagnosis. The computer based simulator can give the trainee operator systematic practice in fault diagnosis which is not possible on the real plant because of the irregular nature and unpredictable occurance of process faults. Different failures will occur with varying frequencies such that trainees may never encounter some whilst others may be encountered very rarely.

Some plants require team work not only between individual operators but between operators and maintenance staff. Some of the more sophisticated process training simulators could be used to allow process and maintenance personnel to study the performance of the plant, identify faults and work together to overcome them, and so improve team working between the shift teams.

The advantages and benefits of using computer based simulator training are numerous and varied. The obvious advantage is that new and existing process operators can be trained in the intricacies of plant operation without risking loss of life or injury to other personnel and/or loss of production due to equipment downtime.

New process units can be brought on-stream earlier since the operators can be trained thoroughly during construction, in conditions exactly like those in the actual control room. The commissioning phase can be shorter since the operators will have rehearsed through simulation(F1).

Plant efficiencies can be improved by training the operators to control the plant within tighter limits. Simulator training enables the quantitative effects of minor changes to process conditions on efficiency and product yield to be demonstrated(F1)

Plant safety can be improved by training operators to respond correctly to emergency situations. The simulator allows the trainee to gain repeated practice in emergency procedures so that when hazardous situations occur on a real plant he is better equipped to respond(M2). The trainee can gain systematic practice in fault diagnosis so improving his diagnostic skills and helping him to recognise earlier the propagation of faults which could lead to hazardous situations.

Training simulation tends to be enjoyable and therefore increases motivation towards learning. The operator's active involvement in the training exercise tends to overcome apathy and indifference. It can improve an operators confidence so that he handles emergency condition's with less stress, and therefore improves his control of the system.

Computer based simulation training has led to three measurable results(D8) :-

(a) Trainees learn fundamentals better when simulation is part of the training programme.

(b) Trainees learn more, such as demonstratable skills in plant start-up, when simulation is a part of the training programme.

(c) Trainees accomplish the above in less time when simulation is part of the training programme.

Simulation training also allows the learning environment to be controlled. The control may be over the degree of complexity of the task that the trainee encounters. For example, the trainee could be given a simple task or parts of the overall task or a general outline of the system before being given the full complexity of the task. The trainee's experience can be structured. Additionally, various forms of feedback can be given to the learner in order to shape and direct his performance(S8). Interactive CBT simulations, in particular enable better feedback to be given on the trainee's actions than would occur if the trainee was being trained on the real plant(D2). It enables precise instructional objectives to be set with appropriate remedial action for trainees who fail to reach the required level.

The learning exercise can also be controlled by changing the speed of response of the simulation. This may be necessary so that trainees make efficient use of their time in training. For example, a start-up procedure may in real life take several hours to complete, various parts of the plant having a slow response to operator inputs. A simulator enables the trainee to experience a range of plant conditions in a much faster sequence than they would be encountered with daily experience on the plant. In other situations where a task involves high speed, practice on a simulator will allow an initial slowing down of the task to enable the response sequences to be learned(S8).

The common disadvantages of simulator training seem to be centred on their design and implementation(M8). Simulations take a long time to prepare and to operate. They require skilful designing, where as trainers in the classroom situation can 'think on their feet' to overcome difficulties, simulations must be pre-planned and pre-packaged catering for all contingencies. There is a danger that trainees may develop an over-simplified view of the real life operating situation and it may be difficult for the trainee to translate simulated experience into his real work situation. Training simulator equipment is very expensive and therefore only severe training problems have justified the use of simulation. However, with the current availability of relatively inexpensive microcomputers and with greater care taken at the design phase there is no reason why training simulation should not find much more widespread use in the process industries since the benefits it can bring are substantial.

Chapter 5 Fault Detection And Diagnosis

5.1 Introduction

The malfunction of plant equipment and instrumentation is a major cause of loss in the process industries. Malfunctions increase plant operating costs and more seriously can cause major accidents such as explosions, so endangering human life.

Himmelblau(H4) defined some terms associated with fault detection and diagnosis :-

Fault or Malfunction in relation to plant equipment is defined as the departure from an acceptable range of an observed variable or calculated parameter associated with the equipment.

Failure is defined as the complete inoperability of plant equipment or the process ie the equipment or an instrument lacks the capability of carrying out its specified function.

Fault Diagnosis is the determination(after detection of the occurance of a fault) of the equipment, or portion thereof, that is causing the fault.

Reliability is defined as the probability that a piece of plant equipment will perform a required function under stated conditions for a stated period of time.

A fault will not necessarily become a failure. Most modern process plants are sufficiently flexible and well organised that as soon as a fault appears in one of the plant's systems, the system automatically compensates for the fault so that continuous operation is maintained.

Early detection and diagnosis of a fault whether by the process operator, or by a computer based diagnostic tool, or a combination of both is desirable to prevent the sudden failure of equipment. Complete malfunction of a piece of equipment is usually relatively easy to detect and diagnose but by the time it has occured considerable damage may have taken place. The failures of plant equipment can often be prevented if the early signs of impending breakdown are recognised.

The early detection of process faults is achieved by monitoring deviations in the process operating conditions. These deviations can be catagorised in terms of particular observations such as :-

(a) Pressure deviations

(b) Temperature deviations

(c) Flow deviations

(d) Level deviations

(e) Excessive vibration of equipment.

In addition other measurable characteristics include :-

(a) Corrosion

(b) Erosion

(c) Fouling

(d) Cavitation

(e) Fluid hammer

(f) Loadings

(g) Expansion

(h) Contraction

(i) Fluid properties

(j) Catalyst activity.

The types of faults which could occur and their expected probability of occurance are difficult to obtain since failure rates and faults depend on the operating conditions and the particular plant's equipment. Some causes of process deviations and hence of faults are given in Table 5.1. Lees(L7) has presented a review of instrument failure data. Trotter(T2) has given a check list of the causes of faults in centrifugal pumps. There is also a databank maintained by the Systems Reliability Service of the UKAEA which provides a library of equipment malfunction information(A2). Access to the databank is available by subscription.

Table 5.1 Causes of Process Faults(H4)

Poor distribution
Improper Mixing
Hot spots
Overheating
Resonances
Stress on bearings and shafts
Improper lubrication
Vortex generation
Blockage
Sedimentation
Adhesion
Surging
Syphoning
Improper design
Leakage
Spillage
Defects in construction
Power failure
Instrument failure
Sticking valves
Catalyst poisoning
Contaminants
Failure to follow operating procedures
Human error
Climatic effects
Materials decomposition

The task of fault detection and diagnosis still mainly centres around the process operator. As the operator carries out his work, he quite unsystematically carries out some alarm scanning and malfunction detection. Much of his effort is usually devoted to preventing production problems. The operator carries out a variety of checks on instruments' readings using his accumulated experience of the past behaviour of the instrument to interpret the significance of off-scale, constant or excessively noisy readings, or readings which do not agree with other measurements. He employs all the human senses of sight, hearing, smell and touch as he continually checks the working of the process equipment. Each operator normally has his own personal set of early warning signals at which he starts to take action to correct a possible malfunction. The role and training of the process operator in fault detection and diagnosis will be discussed further in the next section 5.2.

Even though the operator usually performs his tasks reasonably well, the tasks can be monotonous and boring and in such circumstances the provision of computer-based aids for routine work has definite advantages. The computer can provide the scanning function tirelessly, imperturbably and speedily. The operator's role in malfunction detection cannot be carried out entirely by computer, but just by taking over the part of the interpretation of off-normal signals the operator will be released to concentrate on more difficult jobs for which he is better suited. A process operator is probably better at those aspects of malfunction detection which require intelligent decision-making such as pattern recognition and the taking of corrective actions which involve manual operations. In this way, a better, more appropriate allocation of tasks between man and the computer can be achieved leading to a more optimum use of both(H4). There are several workers developing analysis techniques for computer-based diagnostic aids but since the objective of this work is to improve the knowledge and skill of the process operator these will only be discussed briefly in a later section 5.3.

5.2 The Process Operator's Role in Fault Detection and Diagnosis

The process operator performs the important task of detecting and diagnosing plant malfunctions in the control room. The detection of faults can be obvious such as serious plant breakdowns which cause alarms to illuminate and a siren to annunciate to indicate the process parameters which are out of tolerance. Alternatively and more importantly, plant malfunctions can be incipient where the fault has yet to give rise to an alarm condition. Instrument malfunctions are one source of incipient malfunctions.

Anyakora and Lees(A3) have investigated the detection of instrument malfunction by the process operator. In general, malfunction may be detected either from :-

(a) The condition of the instrument, or

(b) The performance of the instrument.

For example, detection from condition is illustrated by observation on the plant of a leak on the impulse line to a differential pressure transducer or the stickiness of a control valve. Detection from performance is achieved by observation in the control room of an excessively noise-free signal from the transducer or of an inconsistency between valve stem position and the measured flow for the valve.

One of the principal detection aids is the chart recorder. Some typical measurement signals traced on chart recorders are shown in Figure 5.1. The operator detects error in such signals by making comparisons and using redundant information such as :-

(a) 'A priori' expectations

(b) Past signals of instrument

(c) Duplicate instruments

(d) Other instruments

(e) Control valve position.

Therefore, considering the displays given in Figure 5.1, it may be expected that :-

(a) An instrument reading will not go 'hardover' to zero or full-scale.

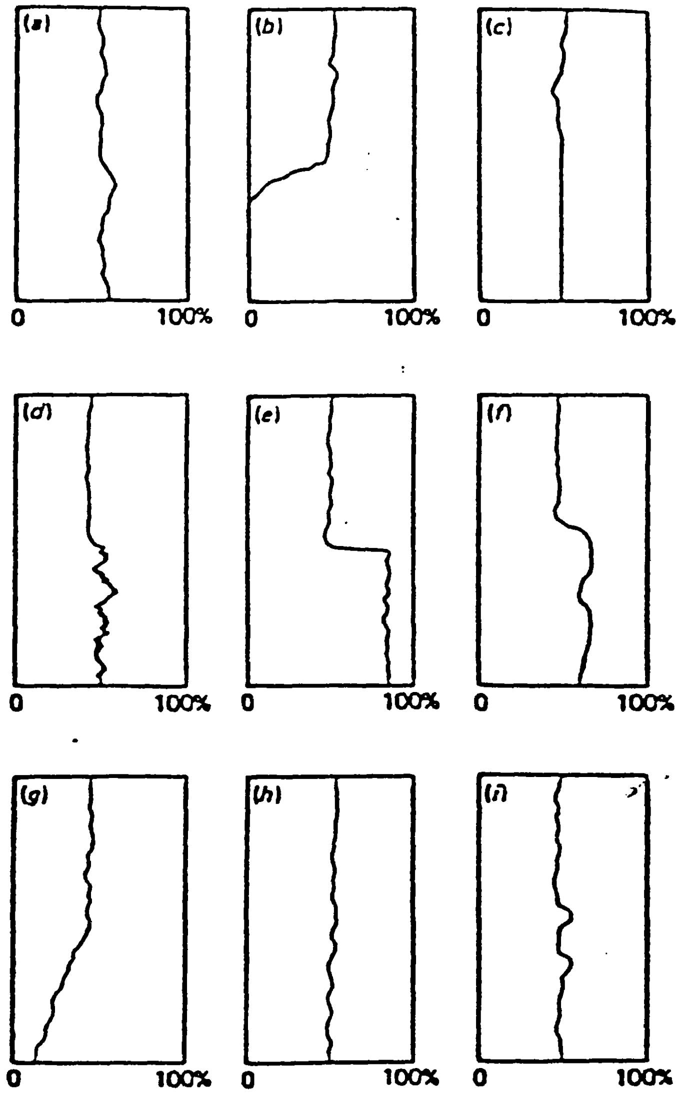
(b) An instrument reading will exhibit a 'live' rather than a 'dead' zero reading.

(c) An instrument reading will exhibit a certain amount of noise.

(d) The rate of change of an instrument reading will not exceed a certain value.

(e) The reading is free to move within the full-scale of the instrument.

Figure 5.1 : Typical Chart Recorder Displays (A3)



(a) Normal Reading
(b) Reading Zero
(c) Reading Constant
(d) Reading Erratic
(e) Reading Displaced Suddenly
(f) Reading Limited Below Fullscale
(g) Reading Drifting
(h) Reading Cycling
(i) Reading with Unusual Features

On this basis, the operator might diagnose malfunctions in any of the displays shown. However, this will vary with the plant operating conditions. For example, during start-up, zero readings may be correct. Some variations of the expectations or some confirmatory checks may be necessary. The level of noise will vary with individual instruments and therfore the operator will have to use his knowledge of the range of variation of noise on a particular instrument in the past. The checks described do not show unambiguously that a particular instrument is not working properly but they do indicate inconsistencies which need to be further investigated.

Marshall and Shepherd(M10) have also investigated the detection and diagnosis of faults and malfunctions by the process operator. They believe that experienced, skilled process operators develop a small number of diagnostic principles which assist him in diagnosing the cause of a plant failure from an array of control panel indications. In general, four basic rules could be followed:-

(a) Scan the control panel to locate the general area of failure.

(b) Check all the control loops in the affected area. Are there any anomalous valve positions ?

(c) High level in a vessel and low flow in associated offtake lines indicates either a pump failure or valve failed 'shut'. If valve Ok then pump failure is a probable diagnosis.

(d) High temperature and pressure in column head associated with low reflux in reflux drum indicates overhead condenser failure provided all pumps and valves are working correctly.

These could be supplemented by further plant specific rules where necessary. Shepherd et al(S1) compared three fault diagnosis training methods, namely diagnosis after training with :-

(a) 'Theory' - Conventional plant description

(b) 'Rules' - Diagnostic rules of thumb

(c) 'No-story' - No prior theoretical instruction.

They concluded that the teaching of conventional theory is of limited value and for versatile diagnostic performance, training should include generalised 'rules of thumb' such as those described.

The diagnostic 'rules of thumb' approach forms the basis of a fault finding training programme for process operators developed by Marshall et al(M11),(M12). The programme consists of three parts:-

(a) Familiarisation training

(b) General diagnosis training

(c) Plant-specific diagnosis training.

These three parts try to ensure that the trainee is competent to :-

(a) Read instruments

(b) Appreciate how instruments monitor and control processes

(c) Recognise and identify the cause of plant failures

(d) Deal with unexpected or uncommon plant failures which require an understanding of the essential physical and chemical characteristics of the process.

The familiarisation training introduces the trainee to the instrumentation in general and to elementary fault diagnosis. The training starts with a slide/tape programme in which the trainees are taught the name and function of instruments commonly found on plant control panels. They practise reading instruments, to note whether values are higher or lower than their setpoints and to interpret valve output positions. A video tape programme of a computer graphics simulation(M6) is then used to introduce the trainee to automatic control and elementary fault diagnosis. It consists of a simple tank level control system which is displayed on the screen with its associated instrumentation using very simple graphics.

The diagnosis training makes use of a simple control panel simulation(D7). The simulated control panel is constructed by mounting printed magnetic tiles which represent individual plant instruments on a large magnetic board. Pointers and labels, similarly made from magnetic tiles, are superimposed on the instruments and these can be adjusted to represent different indications. Simulated control panel indications are photographed for each fault and the slides produced are back-projected and enlarged to life size. This allows the trainee to make rapid comparisons between closely related faults and allows him a great deal of practice in a relatively short time.

The general diagnosis training introduces the trainee to the general principles of diagnosis by making use of a simulated plant and a range of typical fault finding problems. The trainees learn to apply the diagnostic 'rules of thumb'. Individual control panel indications are withheld from the trainee until requested so that the instructor can encourage the use of the 'rules' and control the way in which information is acquired(M13).

The plant-specific diagnosis training utilises the same simulation equipment to produce faults specific to a particular plant. The trainees are encouraged to apply the diagnostic 'rules of thumb' to actual process faults which they are likely to encounter on the real plant. Marshall et al(M11) describe the plant-specific training implemented at ICI Nylon Works, Wilton to train a team of operators on the Cyclohexane Oxidation Section.

5.3 Computer-Based Diagnostic Aids

Computer-based diagnostic aids could be made available to the process operator either via an existing process control computer or an off-line microcomputer. Himmelblau(H4) has produced a comprehensive review of the many potential analysis techniques available to the engineer in developing a computer-based diagnostic aid. These methods include :-

(a) State and parameter estimation

(b) Pattern recognition.

State and parameter estimation techniques require the existence of an accurate mathematical model of the process. The general information flow is shown in Figure 5.2. A series of measurements is made, either periodically or continuously, of the observable process responses. The process inputs are used in a mathematical model to predict the process state variables and coefficients. These can then be compared via statistical tests with reference values to ascertain if faults exist. In some instances, faults can be detected by relating the model parameters to physical features of the process such as utilising material and energy balances.

Pattern recognition is the process of assigning a label or category to a pattern of data on the basis of certain features in the pattern. This can be achieved by comparing a set of process data with existing templates to determine which template has the closest match and hence identify the fault which is causing the particular pattern.

Figure 5.2 : Information Flow for State and Parameter Estimation (H4)

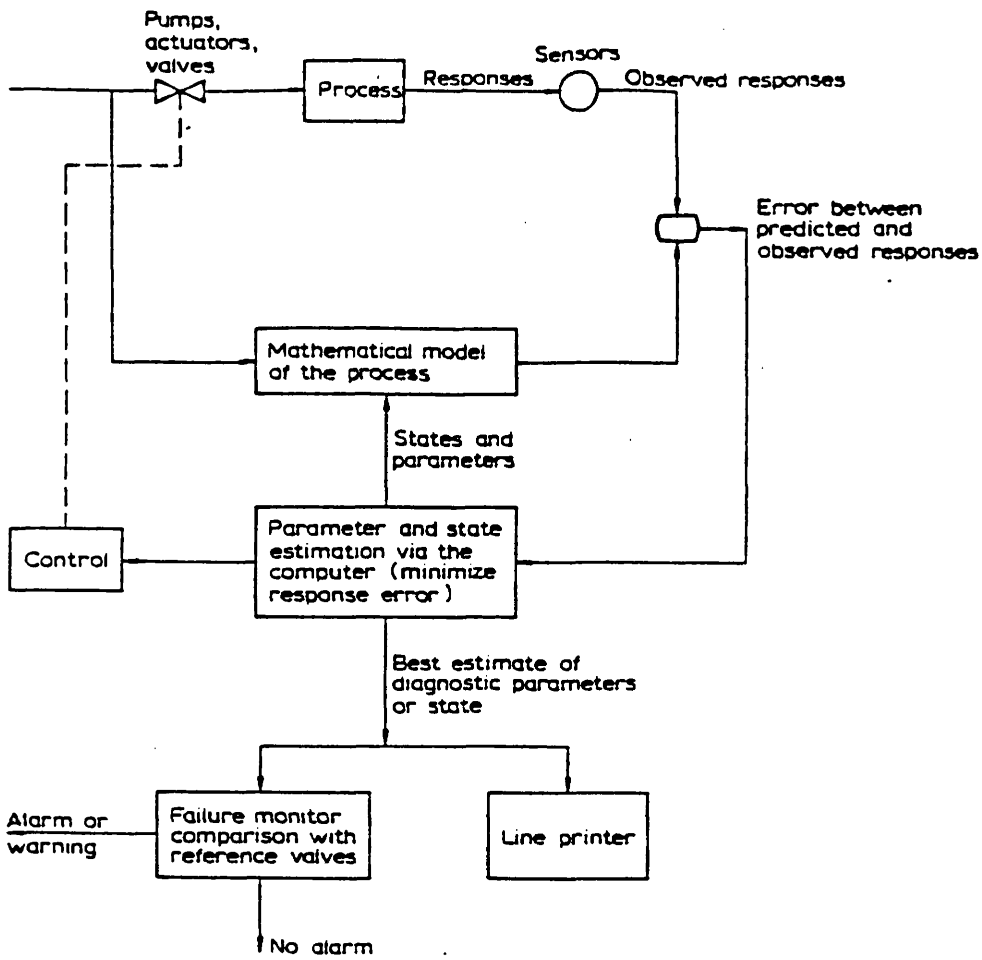
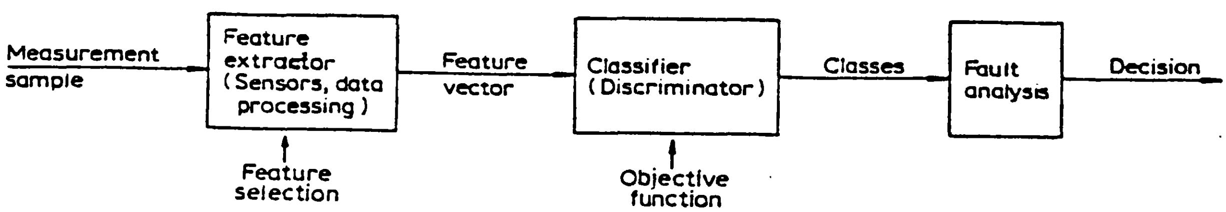


Figure 5.3 : Pattern Recognition Procedure (H4)



Alternatively the pattern can first of all be simplified by feature extraction and classification(H4). This is a three stage process as shown in Figure 5.3. First of all, process measurements such as temperature, pressures, concentrations and flowrates are made. Selected features of these measurements are computed or isolated and combined into a feature vector. Next, various decision rules are applied to the feature vector to classify it into one or more classes such as normal operation, fault condition 1, fault condition 2 etc. Finally analysis of the feature vector can take place to determine the cause of the fault.

There are a number of methods of holding the cause-effect information required for the templates and the analysis of the feature vector. These methods include(A4) :-

(a) Failure modes and effects analysis(FMEA)

(b) Hazard and operability studies(Hazop)

(c) Fault trees

(d) Event trees

(e) Cause-consequence diagrams.

In FMEA the failure modes of a component are listed together with the effects of each failure mode in a tabular format. In a Hazop study for a continuous process plant the deviations of the variables(flow, level, pressure, temperature, concentration) are considered systematically and the causes and effects of these deviations are developed and again recorded in tabular form.

In a fault tree the fault which is to be investigated is taken as the top event of the tree and the tree is developed in terms of the cause events and the logical relations between these events. The information given in fault trees can also be represented as truth tables or by Boolean algebra. In an event tree the fault is taken as the bottom event of the tree, and the tree is developed in terms of the consequence events and the logical relations between these events. In a cause-consequence diagram the fault is taken as the critical event, and the diagram is developed in terms of the cause event and the consequence events and the logical relations between these events. The time order of these events is also taken into account.

One very useful computer-based aid for the process operator would be an on-line alarm analysis facility. This should be able to assist him to order and interpret the alarms as they occur in real time so that several alarms are shown to be part of a sequence caused by the same prime cause alarm. Alarm analysis makes use of a form of the fault tree called alarm trees. They are less rigid than fault trees with no predefined top event and they describe the interactions between the various alarms available on the plant.

Lees(L8) and his co-workers are developing a systematic, or algorithmic method of creating a fault propagation structure in a process control computer which can then be interrogated in real time as alarms occur. The work has resulted in two methods of alarm analysis(L9). In both the input data are the system topology and a simple model or set of models for each unit operation. The first method involves the creation of a loosely-structured network of the process variables and then a network of the process alarms. The alarm network, which maybe created off-line, constitutes the fault propagation structure and is stored in the process control computer. It is then interrogated in real time as the alarms occur to give alarm trees. In the second method the input data are stored in the process control computer and when alarms occur a fault tree for the top event is synthesised in real time using the data. There is no prior processing of the input data as in the first method.

A further computer-based diagnostic aid useful to the process operator could be the application of expert systems(A5),(A6). An expert system is simply a computer program which is able to emulate an 'expert' to give advice on problems of a specific type. The system formulates its advice on the basis of data for the 'domain' of the system provided by the 'expert'. The data are normally 'rules' which can be modified or replaced as knowledge about the domain is accumulated. The expert system is capable of explaining its line of reasoning to the user in terms of the rules it has used. The system works by asking the user a series of questions relevant to the problem. In a well defined system the questions rapidly become specific to that part of the domain in which the particular problem lies. The system provides a possible framework for process plant fault diagnosis from alarms and/or other indications. The information contained within fault trees and cause-consequence diagrams can be built up as 'knowledge' within the expert system. Andow(A5) illustrates the possible use of such systems with a simple tank level example.

5.4 Discussion

Fault detection and diagnosis is a key skill which the process operator seldom has the opportunity to practise. It was stated in Chapter 1 that the main objective of this work was to develop methods of simulating chemical plant operation to achieve process personnel training objectives. Therefore, it is important that these training simulations include the opportunity for the trainee to practise and develop his fault diagnostic skills.

The work of Himmelblau(H4) and Anyakora and Lees(A3) will be useful in selecting typical process and instrumentation faults to include in the generic simulations. The 'rules of thumb' developed by Marshall and Shepherd(M10) for process faults and Anyakora and Lees(A3) for instrument faults are worth presenting to the trainee so that he can use these as the basis for developing his own set of heuristics for fault diagnosis. Chapters 7 and 8 present a number of examples of training simulations which include fault diagnostic exercises.

Chapter 6 Computer Simulation of Plant Operation

6.1 Introduction

This chapter considers the development of microcomputer-based interactive simulations of plant operation for use in plant personnel training. It should be remembered that the simulation must satisfy training objectives as outlined in Chapter 2 and section 4.2 of Chapter 4. This will affect the simulation's development when compared to simulations developed for other purposes such as design and analysis.

The selection of suitable microcomputer hardware and software for producing interactive simulations will be discussed in the next section 6.2. Section 6.3 considers the development and structure of interactive simulation programs and the production of the required mathematical model will be discussed in section 6.4. Section 6.5 discusses a number of considerations which need to be taken into account when developing interactive simulations.

6.2 Microcomputer Systems for Interactive Simulation

When using a microcomputer for training, a much higher degree of user interaction is required than is necessary when using the machine for other purposes such as engineering calculations. Good text and graphics, preferably in colour, are desirable so that the results of simulation calculations can be dynamically displayed on the screen, perhaps using an animated mimic of the plant control panel. The trainee's keyboard skill cannot be assumed and so other means of interaction should be available such as a touch screen or a mouse.

The software must allow you to be able to(B2) :-

(a) develop text and graphics to produce a dialogue with the trainee,
(b) match trainee answers for question judging during tests,
(c) evaluate trainee performance,
(d) direct trainee to relevant modules based on performance,
(e) produce mathematical models to simulate plant processes to a sufficiently high degree of fidelity,
(f) control peripheral devices such as slide/tape machines.

It must be fairly easy to program, to allow a reasonable production of courseware for non-computer specialists. The instructional simulations need to be written in a dynamic, interactive fashion to allow the trainee to take an active role which has been proved optimal for learning(B3).

The application of several microcomputer systems to interactive simulation is described in Appendix 1.2. In particular, the use of the BBC model B, Sinclair QL and Apple II with the 'BASIC' language is described in Appendix 1.2.1. All three systems suffer from fairly poor graphical display facilities and from limited user interaction. The 'BASIC' language allows the mathematical model to be produced easily but enables only simple interaction via keypresses to be used and is clumsy in setting up an instructional dialogue with the trainee.

The IBM PC series of microcomputers offer a more attractive environment on which to produce interactive simulations since they can utilise a variety of graphics cards to produce a number of colour graphics displays from low to high resolution. High level scientific languages such as 'FORTRAN' do not allow graphics facilities to be used. The 'BASIC' language could be used but again it would be difficult to create a good instructional dialogue with the trainee and 'BASIC' does not allow you to use the higher resolution graphics cards which are available.

However, there are languages available for the IBM PC which do allow high resolution graphics cards to be used, mathematical models to be programmed and instructional dialogues to be created. These are called authoring languages and are specialised programming languages which are designed for creating computer-based-training packages(M15).

Appendix 1.2.2 describes the use of the TenCORE authoring language for producing an interactive simulation of a simple tank level control system. A good instructional dialogue is created with the trainee, feedback being given on his actions as he operates the simulation.

The most attractive environment on which to produce interactive simulations is one which has been developed specifically for computer-based-training applications. One such system is MicroTICCIT which is described in Appendix 1.2.3. MicroTICCIT runs on a local area network of IBM PC's or compatibles with a Data General microECLIPSE minicomputer as a host unit. The initial capital cost of the system is high due to the necessity of the Data General host unit and the use of the system has been limited almost entirely to North America.

Another such system is the Regency R2-C microcomputer which is described in detail in Appendix 1.1. One very important feature of the Regency R2-C is the extremely powerful graphics capability which is not matched by any other microcomputer-based training system. The quality and capability of the graphics together with the touch sensitive screen, make the system highly attractive and ideally suited to a high level of interactive simulation(B1). In addition, Regency uses a high level authoring language called 'USE' which provides a framework on which an efficient instructional dialogue can be constructed with the trainee.

Mathematical models can be created easily and efficiently and 'USE' contains many of the features contained within advanced scientific languages such as 'FORTRAN77'.

The Regency R2-C microcomputer system was chosen by management at ICI's Severnside works to deliver computer-based-training material to their workforce. The interactive simulations presented in this work were developed using the 'USE' language and implemented on this machine.

6.3 Program Development and Structure

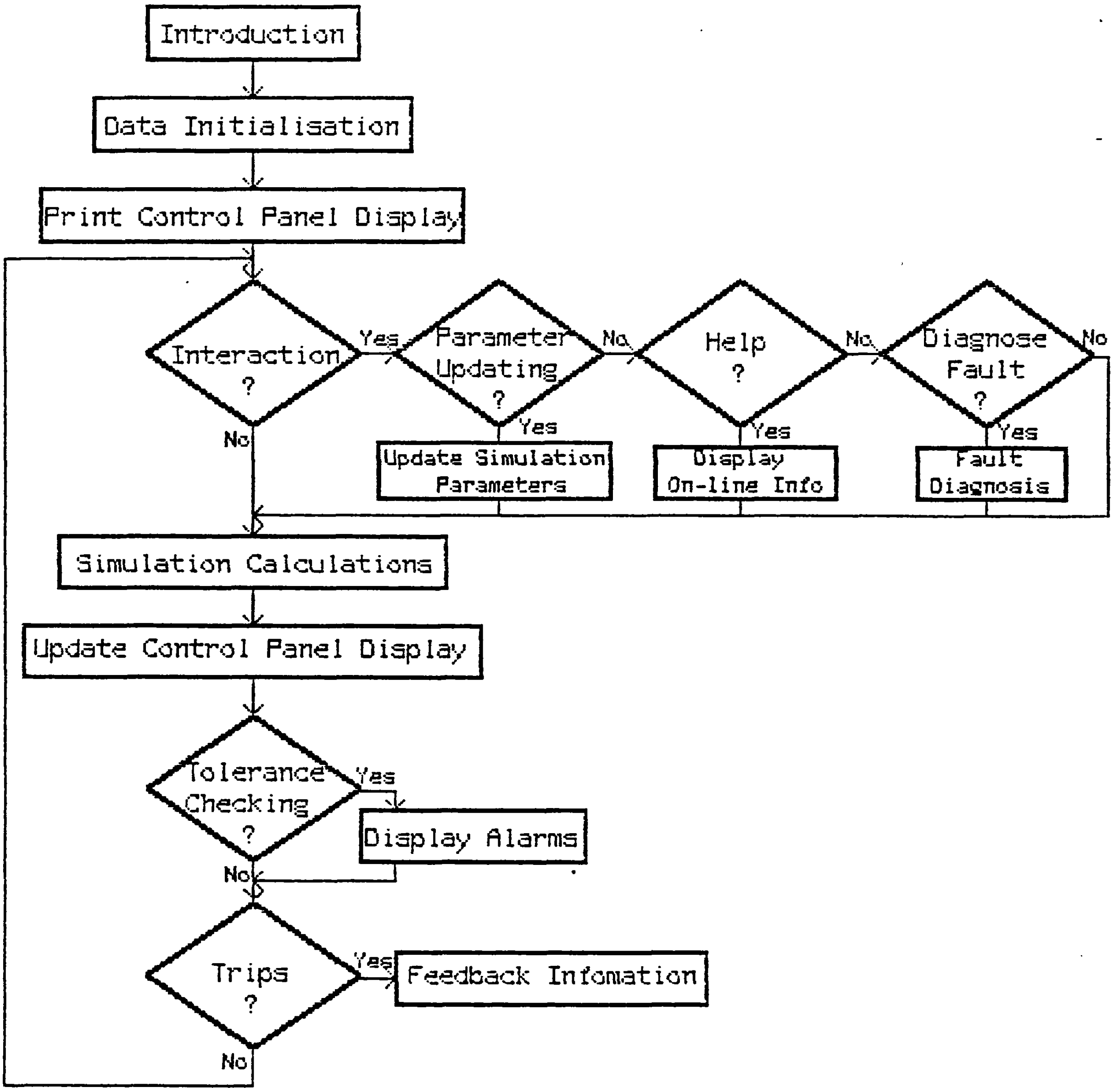
The design procedure of training simulations was described in Chapter 4, section 4.2. In this section the development and structure of the microcomputer-based training simulation programs presented in this work will be described. Table 6.1 lists nine events of instruction which must be considered if a training objective is to be achieved. These are events external to the trainee which are designed to support the internal processes of learning. When selecting the instructional features to be built into the interactive simulation program these events should be considered since they are the main way of influencing the trainee's ultimate behavior.

Table 6.1 Events of Instruction(G4)

1. Gaining the trainee's attention.
2. Informing the trainee of the objective.
3. Stimulating recall of the trainee's prior learning.
4. Presenting to the trainee stimuli with distinctive features(e.g. exaggerate pertinent target characteristics for a novice)
5. Guiding learning.
6. Eliciting performance from the trainee.
7. Providing informative feedback.
8. Assessing performance.
9. Enhancing retention and learning transfer.

For efficient development and operation, all simulation programs should be controlled by a main executive routine. This executive should call all the other subroutines that make up the program. The general executive and hence the structure of the programs presented in this work is given in Figure 6.1. The 'introduction' block 'sets the scene' for the simulation which is to follow. It should present the objectives of the training exercise to the trainee. It should describe the content of the simulation and pay particular attention to the plant or the section of plant being simulated. It should introduce the parameters which the trainee is going to manipulate and the procedures which he is going to follow.

Figure 6.1 : General Interactive Simulation Program Structure



Clear, concise, directions should be given as to how the trainee is to interact with the simulation and to how he can obtain 'help' whilst running the program. The inclusion of 'on-line help' facilities is very important so that the trainee does not have to remember the simulation operating instructions.

The simulation parameters are then initialised and the control panel display printed on the screen. The powerful Regency graphics facilities are used to produce animated mimics of the actual control room instrumentation. Each simulation display contains only the instruments required for the section of the plant being simulated. The relative positions of the instruments on the mimic screen display should be the same as the actual plant. The animated mimics of the individual instruments should also resemble the actual control panel hardware as much as possible. The layout and design of the instruments are important since they affect the strategies which the operator may adopt in seeking information. If the number of instruments required does not fit on one screen display then Regency's four-screen memory is used to store a number of control panel displays which can then be called up in turn by the trainee.

The program then enters the main simulation loop. The 'interaction' block tests for user interaction with the program via the touch sensitive panel or the keyboard. The touch sensitive panel is used for all interactions with the control panel instruments. The trainee has to select the controller he wishes to change by touching the individual controller display on the screen. Then, to make a change, the trainee selects the magnitude of the required change from a menu displayed at the bottom of the screen. This attempts to replicate the control room thought processes where the operator selects the controller he wishes to change and then makes his change. In some programs the trainee can also introduce random faults and disturbances into the simulation and then go through the process of diagnosing their cause. Trainee interaction with the keyboard is reserved for functions which suspend the simulation and provide some other form of instruction such as the 'on-line help' facility and the diagnosis of faults.

The program then updates the simulation parameters based on the trainee's interaction. The next block carries out the simulation calculations which model the operation of the plant. Mathematical modelling will be discussed in the next section 6.4. The animated control panel display is then updated to display the results of the simulation calculations in a form familiar to the trainee. The integration of the 'interaction', 'simulation calculations' and 'update control panel display' blocks has to be carefully structured and this will be discussed as one of the design considerations in section 6.5.

A check is then made on the process parameters to see if they are within set tolerances and alarms are displayed on the screen if necessary just as would happen on the real plant. If the process parameters are at the extreme of the tolerances then the simulation is tripped and the trainee is given feedback information on his actions. Otherwise, the program returns to the top of the simulation loop and checks for user interaction once more.

The provision of good, comprehensive feedback is important since it ensures that the program can be used for individualised instruction without the presence of a training instructor. This 'extrinsic' feedback can be used in a variety of ways. Sometimes trainees will be permitted to make mistakes with the simulation providing either concurrent or terminal feedback. In the former case, the trainee will be given guidance to follow the correct path at each step. In the latter the trainee's mistakes are allowed to build up and feedback is given on failure. This unique feature of feedback through interactive simulation is especially useful in guiding trainees through fault diagnosis. The level of guidence given can be gauged according to the performance and requirement of the trainees(B1).

A number of routines have been written in the 'USE' language to produce the simulations presented in this work. These routines, which include methods for solving equations, models of process control system components and routines to produce animated mimic displays of control panel instrumentation, have been collected together into a package called 'simpac'. A copy of the 'simpac' manual which gives detailed information on each of the routines is given in Appendix 2.

There are several points to consider when developing the overall simulation program and these will be discussed in section 6.5. The mathematical model is the 'heart' of any training simulation programme and so its development will be described in detail in the next section, 6.4.

6.4 Mathematical Modelling

6.4.1 Types of Mathematical Models

The simulation of the operation of chemical plant involves the derivation of a mathematical model of the process. These models will contain equations which are made up of dependent variables such as flow, composition and temperature and independent variables such as time and position in a particular vessel. The models can be classified in a number of ways(H4) : -

(a) Linear vs nonlinear
(b) Steady-state vs unsteady state
(c) Lumped parameter vs distributed parameter
(d) Deterministic vs stochastic
(e) Continuous vs discrete-event.

(a) Linear vs nonlinear.

Equations and hence, mathematical models are linear if the dependent variables or their derivatives appear only to the first power. Each term in each equation of the model should be examined and if any of the terms has a power not equal to one then the entire model is nonlinear. In practice, the ability to use a linear model for a process has great significance, since the solution of the equations of linear models is an order of magnitude easier than the solution of nonlinear ones.

(b) Steady state vs unsteady state.

Steady state refers to a process which is functioning but in which the point values of the dependent variables remain constant. Unsteady state processes represent the situation where the process dependent variables change with time. An example of an unsteady state process is the start-up of a distillation column which would eventually reach a pseudo steady state set of operating conditions. If this was examined in more detail, the column would actually be operating in the unsteady state with minor fluctuations in temperature and composition, for example, taking place all the time, but ranging about 'average steady state' values.

(C) Lumped parameter vs distributed parameter.

A lumped parameter representation of a process means that the spatial variations are ignored and that the various properties and the state of the system can be considered to be homogeneous throughout the entire system volume.

A distributed parameter representation, on the other hand, takes into account the detailed variations in behaviour from point-to-point throughout the system. All real systems are distributed in that there are variations throughout them but as the variations are often relatively small they may be ignored and the system assumed to be 'lumped'.

Lumped parameter modelling can be used where the response of a process is for all practical purposes instantaneous throughout the process. If the response shows instantaneous differences along the vessel, then it should not be 'lumped'. However. since the solution of lumped parameter models is significantly simpler than the solution of distributed parameter models, the latter can often be approximated by an equivalent lumped parameter system. An example of a lumped parameter model is a mixing tank. Calculations are usually based on the assumption that the tank is perfectly mixed so that the entire volume of the tank consists of a homogeneous material that is the same as the outflow. In the real tank, there will be baffles and corners where the mixing will not be perfect but these varations are usually ignored in favour of some overall average values for the properties in the mixing tank. For many purposes this works quite well but for some chemical reactions, for example, the nonideal mixing effects may become important.

(d) Deterministic vs stochastic.

A deterministic model is one in which each variable or parameter can be assigned a definite fixed value, or series of fixed values, for a given set of conditions. A stochastic model is one in which the variables contained in the model show random variations. In practice, certain parts of a mathematical model can be deterministic such as the prediction of physical properties but the overall process model will always be stochastic since a given random input will yield a corresponding random output.

(e) Continuous vs discrete-event.

Continuous models contain variables that change in a continuous manner with respect to one or more independent variables. In the simulation of chemical plant operation the independent variable is usually time. The model will comprise a set of ordinary differential equations which describe the time dependency of the process variables. Discrete-event models are also time-varying models but in which the state of the system is regarded as remaining essentially unchanged between each discrete-event. Time advances in a discontinuous fashion from event to event.

Continuous and discrete-event models can also be combined. For example, the simulation of batch reactor operations involves the reactor being charged with fluid ready for reaction, a continuous process. A small time period could then follow before the reactor is heated to initiate the reaction. This small time period is a discrete-event.

The subsequent generation of the product by reaction over a period of time, is another continuous process.

It is possible to use a number of different types of mathematical model for training simulations. The selection of which type to use will be governed by the objectives of the desired training. For example, if the dynamics play an important part in the simulation such as in teaching the operation of process control systems, then a model which reproduces these dynamics should be used. If, on the other hand, the objective is to demonstrate the inter-relationships between process variables, then a model which represents these 'cause and effect' relationships should be used. These two approaches will be discussed in the next two sections, dynamic simulation in section 6.4.2 and 'cause and effect' simulation in section 6.4.3.

6.4.2 Dynamic Simulation

Dynamic simulation can be achieved by using continuous models with either lumped or distributed parameters. The lumped parameter approach results in a model where time is the only independent variable and the dependent variables, such as concentration and temperature, represent overall averages throughout the entire volume of the system. In effect, the system is assumed to be sufficiently well mixed so that the output concentrations and temperatures are equivalent to the concentrations and temperature within the system. In general, applying the laws of conservation of mass and energy the lumped parameter approach gives rise to equations of the form :-

Rate of accumulation or depletion within the system	=	Rate of transport into system through system boundary
	-	Rate of transport out of system through system boundary
	+	Rate of generation within the system
	-	Rate of consumption within the system

The equations which result are a set of ordinary differential equations. The set of equations describe the variation of the process variables with time. The independent variable, time is common to all the equations contained in the set. The solution of the equations starts from a defined initial condition and continues in increments of time until the simulation is stopped. The equations may be solved analytically or numerically. However, analytical solutions are confined to fairly simple sets of equations and therefore the numerical approach is favoured in this work.

A number of dynamic simulation packages which would enable these equations to be solved were mentioned in Chapter 2. However, this work does not require the aid of a sophisticated simulation package since the aim is to produce a practical representation of plant operations to enable training objectives to be satisfied. Therefore, relatively simple simulation modules have been written, making use of numerical integration routines written in the 'USE' language. These routines are described in detail in the 'simpac' manual in Appendix 2.

It is sometimes necessary to consider the physical parameter variations with respect to space within a system, particularly when using simulation for design and analysis. Distributed parameter models result in sets of partial differential equations which are more difficult to analyse mathematically. However, it is possible to represent distributed parameter models by a series of lumped parameter approximations. This is particularly useful when deriving training simulations since the mathematical model does not have to be as accurate as a model used for design and analysis. For example, the variables in a heat exchanger depend on time and their position in the exchanger. In some cases, the exchanger can be represented by a series of lumped parameter approximations which account for the spatial variations along the exchanger's length. This approach has been used for the generic heat exchanger simulations presented in Chapter 7.

The ordinary differential equations produced by lumped parameter models can also be converted into transfer functions using the Laplace Operator of the form(F4) :-

$$\frac{\text{Input}}{\text{Output}} = \frac{G}{\tau s + 1} \qquad \text{1st Order}$$

$$\frac{\text{Input}}{\text{Output}} = \frac{G}{\tau^2 * s^2 + \tau \zeta s + 1} \qquad \text{2nd Order}$$

The conversion requires a lot of algebraic manipulation to arrange the equations in the correct form. It produces a transfer function for each output variable in terms of each input variable. This approach becomes increasingly complicated as the number of inputs and outputs increases. However, the transfer function approach is very useful for modelling the individual elements of process control loops. For example, measuring elements such as thermocouples contained in thermowells can be modelled so that the measured variable, temperature is related to the actual fluid temperature by a first order transfer function(F4).

Since ordinary differential equation process models can be converted into first and second order transfer functions it is reasonable to assume that actual plant transient data could also be fitted to such transfer functions to produce an empirical model of the process. This approach requires the studying of process reaction curves(C7). These are experimentally obtained plant transient curves produced by forcing functions such as impulses, steps or sinusoids. By analysing the curves, values of the gain, time constant, and damping factor for first and second order transfer functions can be obtained. Lees and Clark(L10) describe the application of this technique in producing a transfer function model of direct fired liquid natural gas vaporisers for use in the analysis of control strategy.

Routines have been developed to numerically solve first and second order transfer function models and these are described in the 'simpac' manual in Appendix 2.

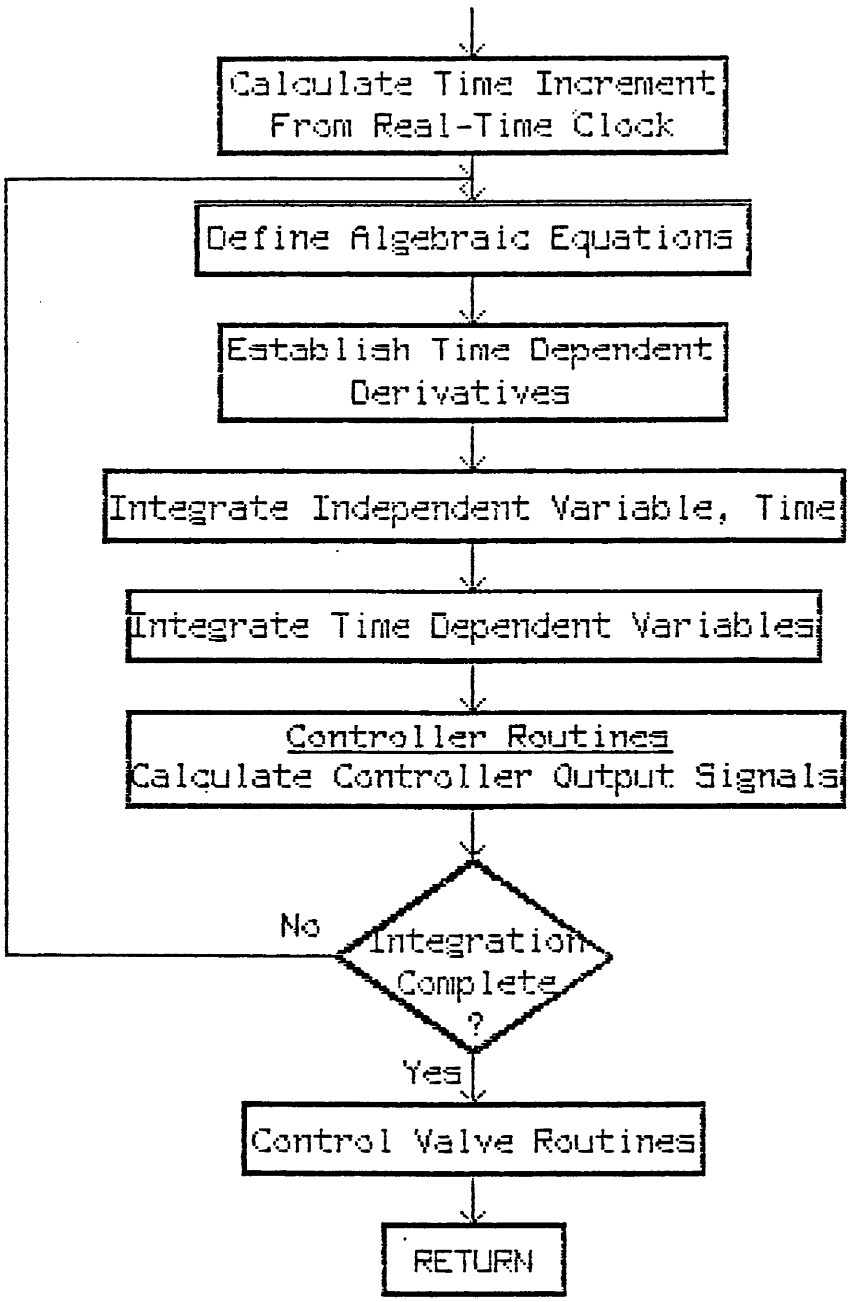
The choice of which mathematical modelling approach to take when producing dynamic simulations for training will depend to some extent on the quantity and quality of the process data available on which to base the model. If process reaction curves are available or can be obtained easily with the help of a 'friendly' plant manager then the use of transfer functions derived from these curves provides a very powerful way of modelling the process. However, the model cannot be used outside of the range of the data used to produce it which may limit it's training effectiveness.

In many plants and in particular those of ICI Severnside studied in this work, there is a great shortage of detailed process data. In this situation it is better to use an ordinary differential equation model of the process since this will be based on the physical and chemical properties of the system. A highly accurate model is not required for training purposes, just one which reproduces the plant responses to a sufficient degree of fidelity so that the training objectives can be achieved. Therefore, a fairly simple ordinary differential equation model is sufficient for many cases. The model parameters such as heat transfer coefficients and controller settings can be 'tuned' so that the performance of the model matches to the limited process variables that are available. Since the model is derived from the physical and chemical properties of the system it can be expected to provide a reasonable prediction for process variables which are not available in the data. In addition, an approximation to the process operating conditions outside the range of data can be obtained from the model although its use should be treated with caution.

Fault diagnostic exercises can also be created by locally rewriting the model to simulate the process at that point, or by redefining input variables, so that abnormal operation is simulated and the changes proceed through the simulation. For example, the 'sticking' of a flow control valve can be simulated by rewriting the mathematical model using Boolean equations so that the equations which model the valve are ignored if this fault occurs. A new valve position will not be calculated for the new controller signal and therefore the valve will appear to be 'stuck'. Secondly, the fouling of a heat exchanger can be simulated simply by lowering the value of the overall heat transfer coefficient so that the rate of heat transfer is reduced.

The general structure of the dynamic simulation calculation routines presented in this work is shown in Figure 6.2. First of all the routine 'realtime' is used to calculate the time increment to be used in the calculations which follow. The algebraic equations are then defined and the time dependent derivatives established. The sequence of equations must be properly ordered so that no variable is used which has not been previously defined.

Figure 6.2 : Dynamic Simulation Calculation Routine Structure



The independent variable, time, is then integrated using the routine 'intin'. This is followed by the integration of the time dependent variables using either of the routines 'intde', 'intstiff' or 'intstif2'. The response of the process controllers are then calculated using one of three routines, 'Pcontr' for a proportional only controller, 'PIcontr' for a proportional + integral action controller and 'PIDcontr' for a proportional + integral + derivative action controller.

A check is then made to see if integration is complete. If so, the program passes to the control valve routines where the action of the control valve to the calculated controller output signal is determined using routine, 'valve'. Otherwise, if integration is not complete, then the program returns to the algebraic equations and calculation is continued. The routines mentioned are described in detail in the 'simpac' manual in Appendix 2. The stability of the mathematical calculations, which is particularly important in dynamic simulation, will be discussed in section 6.4.4.

A number of dynamic simulations of plant operations which incorporate fault diagnostic exercises have been written as part of this work. Several generic simulations of individual plant unit operations are presented in Chapter 7 and two plant specific simulations are presented in Chapter 8.

6.4.3 'Cause And Effect' Simulation

'Cause and effect' simulation can be used where the dynamics of the process are unimportant. For example, the dynamics are not important when teaching the effect of changes in feed quality on the product produced by a plant. This requires just a steady state representation of the inter-relationships between these variables. Each steady state can be considered to be a discrete event since the time-dependent dynamics of how the process changes from one steady state to another are ignored. There are two approachs which could be used :-

(a) Database Interpolation

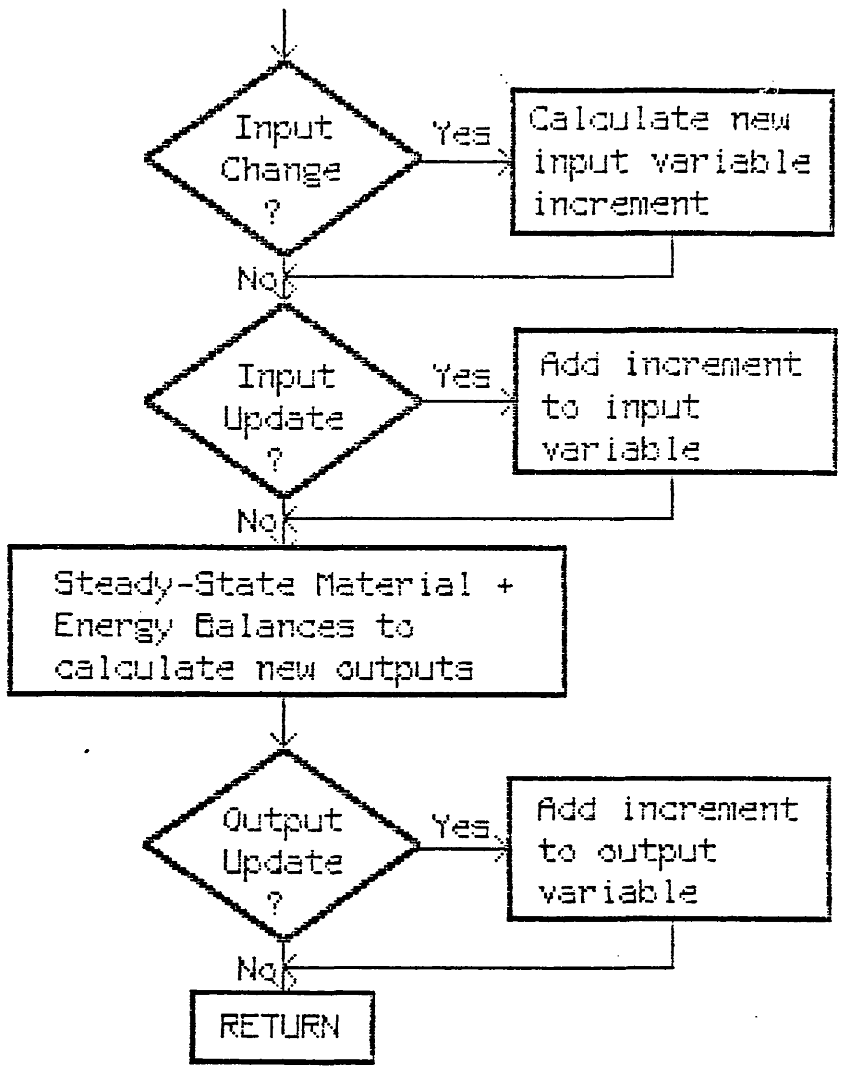
(b) 'Steady State Snapshots'.

Database interpolation can be used when there is a large amount of steady state process data available which covers all the variables that are required for the given training objectives. The approach requires a database to be built up which includes all the necessary process variables together with their values at all the possible conditions encountered by the training simulation. Values of the process variables are extracted from the database using interpolation methods as required. This is a useful approach since it uses actual plant data to model the inter-relationships in the process and therefore produces very accurate predictions of plant steady state conditions.

If the data available is limited, then the steady state material and energy balances should be used to predict the plant inter-relationships. For example, if the trainee makes a change in one of the input flowrates then the material and energy balances will predict the new steady state. The results of these calculations could be displayed on an animated mimic of the control room instrumentation so that the trainee observes the changes in a similar way to that on the plant. However, if the trainee makes a large change in the flowrate then a dramatic change in the steady state variables will result. It is advantagous for training purposes that the effect of the change is broken down into smaller changes, each one a new steady state, so that the overall changes proceed much slower. This approach essentially takes 'steady state snapshots' of the process dynamics.

This approach has also been used in the present work. The general 'steady state snapshot' calculation routine structure is given in Figure 6.3. First of all a check is made to see if the required value of one of the input variables has been changed. If so, then a new increment to add to the current steady state value is calculated. Then a check is made to see if the input variables are at their required values and if not, then the increment is added to the current input value.

Figure 6.3 : 'Cause and Effect' Simulation Calculation Routine Structure



The steady state material and energy balances are then carried out. A check is then made to see if the output variables are at their calculated steady state values. If not, an increment based on the current and calculated values is added to the current output value.

The calculation of the increments to add to the input and output variables can be used to reflect the different speeds of response of the process. For example if the value of a particular variable changes quickly on the actual plant then a large increment can be added to the current value each time so that the required or calculated steady state is reached quickly. Alternatively, if a particular variable changes slowly on the actual plant then a smaller increment can be used. Although this does not model the actual dynamics of the process, it ensures that the simulation retains a 'feel' for the relative speed of response of the individual variables.

'Steady state snapshot' simulations of two actual plant operations have been developed in this present work and they are presented in Chapter 9.

6.4.4 Mathematical Stability

The stability of the mathematical calculations is very important when developing a training simulation. The simulation must have a high degree of 'robustness' so that whatever change the trainee makes the simulation does not 'hang' or go unstable and therefore destroy the trainee's confidence in the instructional program. There are two particular mathematical computations which could cause problems and these are the numerical solution of ordinary differential equations and calculations which require an iterative solution.

The numerical solution of an ordinary differential equation will be stable if the propagated error is bounded. The stability depends on both the numerical method employed and on the nature of the differential equation to be solved. The total error is made up of errors inherent in the solution method being used and errors due to the fact that computation is carried out to a finite precision. The two kinds of error are called :-

(a) Truncation Error

(b) Round-off Error.

Truncation error is the difference between the true solution and the one calculated numerically assuming that all arithmetic operations are performed exactly. These errors may accumulate on repeated integration but Franks(F4) points out that the nature of many chemical engineering problems is such that there is a tendency for these errors to cause slight changes in the calculated derivatives which in turn diminish the resulting truncation errors. This is due to the inherent self-stabilisation which is typical of natural phenomena.

Round-off error is caused by the fact that numbers are represented inside the computer by only a finite number of digits. Although the round-off errors are small, the relative errors can be quite large. If there are numerous steps in the procedure then these small errors can accumulate into large errors. Generally as the time increment is decreased the truncation error of the method decreases but this causes the number of computational steps to increase which causes the round-off error to increase. Therefore, some optimum time increment will exist for which the total error is a minimum. If the numerical method and/or the ordinary differential equation is complex then there will be many computations and many opportunities for error(F5).

This work is concerned with the realistic simulation of chemical plant operations. The rate at which the simulation parameters are updated is fixed by the actual dynamic response of the plant being simulated. Therefore the time increment used in the numerical solution method should enable the time taken to execute one complete loop of the simulation program to be comparable with the actual dynamic response of the plant.

The accuaracy and therefore, stability of the mathematical calculations can be improved by using a higher order solution method to reduce the truncation error. The dependent variable integration routine, 'intde' presented in the 'simpac' manual in Appendix 2 contains five integration methods :-

(a) First Order Euler

(b) Second Order Adams-Bashford

(c) Second Order Runge-Kutta

(d) Third Order Runge Kutta

(e) Fourth Order Runge Kutta.

Each higher order method splits the time increment into increasingly smaller sub-increments in order to carry out the particular solution method. However, the higher the order of the method the more computation steps are required for solution and therefore the round-off errors could start to have an effect. In addition, limitations may be reached if there is a large number of equations to be solved since the time taken to solve the equations may be longer than the time increment required to maintain 'real-time'. 'Real-time' will be discussed as one of the design considerations in section 6.5. Howe(H6) has studied a number of integration methods and concluded that for 'real-time' solution that the second order Adams-Bashford method allows the largest time increment to be used for a given accuracy requirement. However, it still suffers from the fact that instability will result if the time increment becomes too large.

Most dynamic simulations of chemical plant operation involve solving sets of of ordinary differential equations. This involves many computation steps and the equations within the set could have a wide range of time constants.

Consider the solution of the simple ordinary differential equation :-

$$\frac{dy}{dt} = \frac{1}{T} y \quad \text{is} \quad y = A * e^{t/T}$$

where T is the time constant of the equation. The ratio of any two time constants is known as the 'stiffness' ratio and is a measure of the stability of the set of equations. The greater the time constants vary, the 'stiffer' or more prone the system is to instability. The equations having small time constants control the stability of the system whilst those with larger time constants control the truncation error. This is in spite of the fact that the fast decaying small time constant component becomes negligible in size. The equation having the smallest time constant determines the maximum time increment which can be used for stability of the resulting numerical solution.

'Simpac' includes two routines for the numerical solution of 'stiff' ordinary differential equations which have been developed by Franks(F6). These routines, called 'intstiff' and 'intstif2' are described in the 'simpac' manual in Appendix 2. They require the differential equation to be rearranged into a specific algebraic format which may not always be possible. In this case, the structure of the simulation calculations routine will have to be modified in order to account for the faster responding parts of the model. For example, using the simple first order Euler integration the overall time increment could be split up into a number of sub-increments. The faster responding parts of the model could then be integrated over each sub-increment with the slower parts of the model only being integerated over the whole increment.

One possible way of avoiding the restrictions described above is to use a variable step method. This involves monitoring the integration error and adjusting the time increment so as to maintain the error within a specified tolerance. This method requires much greater computer time per solution than the direct methods above. Since the simulations presented here are restricted by external influences which fix the overall time increment the variable step method is unattractive since the number of computations for each time increment would also vary. There is only a finite number of computations which can be carried out for each time increment so that 'real-time' is maintained. However, should greater microcomputer power become available then serious consideration should be given to the use of variable step methods.

The other mathematical operation which could cause problems is the use of iterative solution procedures. It is essential that these do not take a long time to converge otherwise they will affect the overall time increment required to maintain 'real-time'. 'Simpac' contains two routines to speed up the convergence process. These are, 'converg1' which uses partial substitution and 'converg2' which uses Wegstein's method for convergence.

Newton-Raphson convergence has also been used for specific applications. The two important variables to ensure 'robustness' are the initial value and the precision to which the convergence is obtained. A good initial estimate is imperative for quick convergence. The convergence criteria should be fixed so that it is 'tight' enough to obtain a sufficiently accurate solution for the input value but it must not be so 'tight' that a lot of iterations are required to obtain the solution. It should be remembered that it is more important that the mathematical model exhibits a high degree of 'robustness' rather than a high degree of accuracy. The accuracy required for training simulations will be discussed as one of the design considerations in the next section, section 6.5.

6.5 Design Considerations

By definition, simulation is the representation of certain features of a real situation to achieve some specified objective(D7). The present objective is to use the simulations as an aid for training process plant personnel. Therefore, the fidelity of the simulation as it appears to the trainee is of prime importance.

There are three main design requirements(W4) :-

(a) The simulation must operate in real-time or faster.

(b) It must be cost effective.

(c) It must be sufficiently accurate to successfully accomplish the training objectives.

It is important that the simulation responses are displayed to the trainee in real-time or faster, that is the simulated instrument response times are comparable with the actual plant instrument response times. A simulation which operates slower than real-time is not capable of realistic training and the trainee will quickly become impatient and frustrated.

The animated mimic of the control panel instrumentation must be updated at intervals. The screen display updating will take a finite time and so the total time taken to update the display, test for interaction by the trainee and carry out the simulation calculations must not be so great that the trainee is watching a 'dumb' screen for long periods. In particular, if an ordinary differential equation dynamic simulation model is used the total time taken, and hence the real-time increment used in the calculations, must not be greater than any of the equation time constants or instability will result. A detailed description of mathematical stability was given in the last section 6.4.4. In the case of large and complex simulations, 'Rate structuring' will need to be applied. This means that the updating of the screen display, testing for trainee interaction and the mathematical calculations should be split up into a number of sections. The individual sections could be the animation of a particular instrument or the modelling of a particular unit operation. The sections should then be structured according to the time taken to execute each section so that a 'smooth' simulation response is presented to the trainee. The approach is shown in Figure 6.4. In dynamic simulations, the structuring should ensure that the real-time increment used in the calculations is approximately constant for each solution of the differential equations and is as small as possible to keep the inherent inaccuracies in using numerical solution techniques to a minimum.

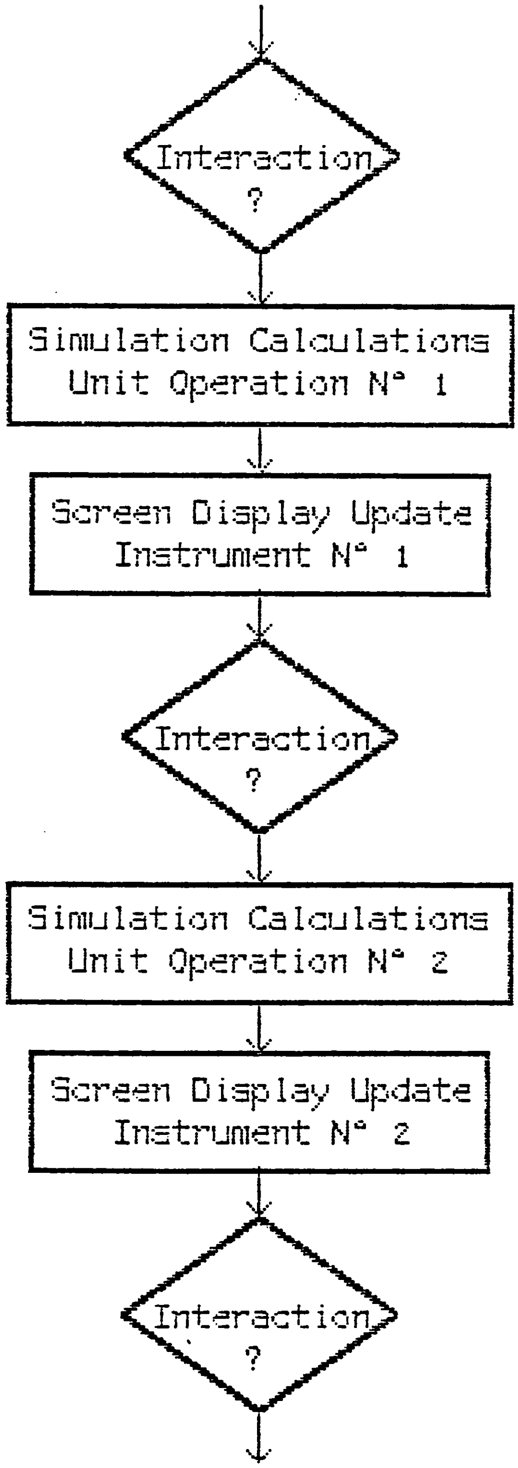
The second and third requirements, (b) and (c), imply that the accuracy of the simulation should be just enough to support the training objectives. In practice, this means that(W4) :-

(a) Only those effects that can be perceived by the trainee should be included in the simulation.

(b) Steady-state system responses should be fairly accurate since large steady-state errors are quite noticeable.

(c) Transient responses need only be qualitatively correct.

Figure 6.4 : Rate Structuring



The amount of realism or the amount of representation of the real task built into a simulation is called the fidelity. Miller(M17) pointed out the relationship between the fidelity of a simulation and the transfer of training value. The relationship is such that as the degree of fidelity increases a point of diminishing returns is reached between the cost of increasing the simulation fidelity and the transfer of training to the real situation. Figure 6.5 suggests that the costs of simulation rise steeply with small increases in fidelity at the top end of the scale. The point of diminishing returns on the graph represents the highest transfer-to-cost ratio after which it costs more to produce transfer value to the task. Therefore, very often, 80% of the benefits of the simulation can be obtained by modelling only a small part of the entire system. It is a good practice to consider how much it is worth paying in order to get the reamining 20% of the benefits(M1).

When considering the accuracy of the simulation, criteria should be used which are based on the effect of the simulation's fidelity on the desired training. Differences between the simulation model and the actual plant's behaviour which do not materially affect the operator's judgment or do not result in an incorrect course of action will have a negligible effect in the training environment. Similarly, differences that occur many hours after the initiation of a transient may be ignored since these differences will never be observed in the training situation.

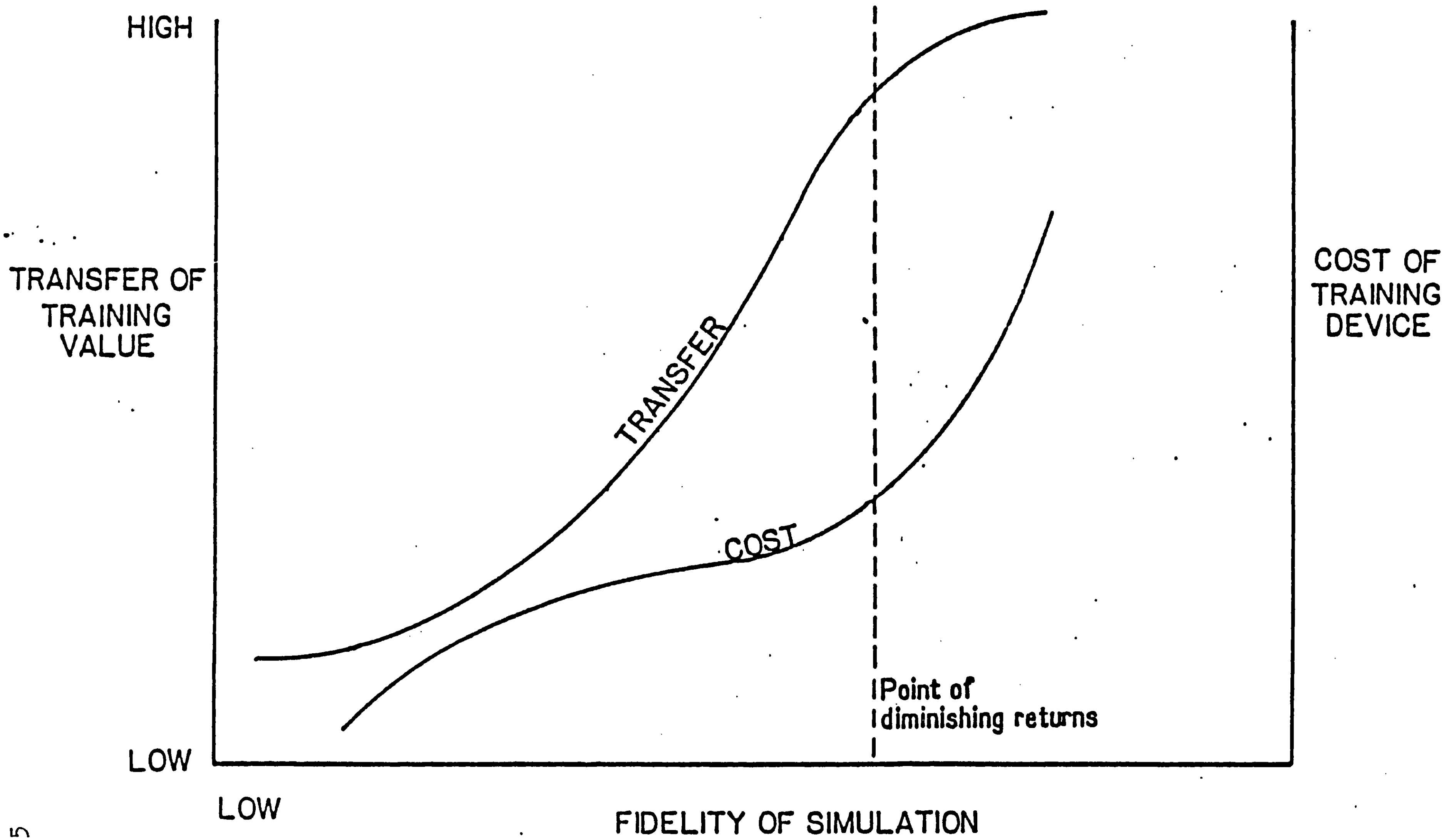


Figure 6.5

The relationship between Cost, Fidelity and Transfer of Training (M17)

The American National Standards Institute/American Nuclear Society Standard No. ANSI/ANS-3.5, "Nuclear power plant simulators for use in operator training" requires that the differences between calculated values of plant parameters and reference plant data should be less than(A7) :-

(a) 2 % for 'critical' parameters

(b) 10 % for 'non-critical' parameters.

In addition, it requires that if a given input produces an alarm or trip on the actual plant then it must also on the simulation and if the input does not produce an alarm or trip on the plant it must also not on the simulation.

The American Standard can be used as a guideline for specifying the accuracy requirements of the simulations presented in this work. It is important that fairly high accuracy criteria are used for the calculated steady state values since the trainee can examine a steady state condition at leisure and in more detail than a transient. It seems reasonable that the calculated steady state values should agree with a set of reference plant data within fixed percentages. The American Standard can be applied so that the 'critical' parameters include the variables which the trainee manipulates and observes directly whilst 'operating' the simulation. The 'non-critical' parameters include those that the trainee cannot directly observe and those that are contained within the mathematical model and are not displayed on the mimic control panel.

This work has used an equation-based approach to producing training simulations since only limited plant operating data has been available. Plant transient tests are costly to arrange, carry out and analyse. Plant ageing such as the fouling of heat transfer surfaces can make the setting up of the simulation to match a particular transient a lengthy procedure. Production schedules cannot be interferred with and safety considerations usually prevent extreme transients, for which training is important, being tried on the plant. It seems reasonable that, for training purposes, the transient responses need only to be qualitatively correct. The simulated transients should not violate the physical laws of nature such as producing heat flow from a cold body to a hot body and they should be accurate in direction and sequence of occurance. The magnitude of the transient is not important as long as it does not give rise to a spurious alarm or trip. However, the resulting steady-state should be accurate within the previously mentioned criteria.

The best people to evaluate the accuracy of the transient responses and the operational fidelity in general are the experienced senior control room operators and supervisors which are found on most plants. They will know the plant responses better than anyone else and will be only too willing to tell you where the simulation is inadequate.

Chapter 7 General Plant Operation Dynamic Simulations

7.1 Introduction

This chapter presents some generic examples of dynamic simulations used for training plant personnel. It uses the ideas presented in Chapter 6. A number of different unit operations together with their associated control systems are modelled to produce a simulation of their operation. The simulations are used to achieve a variety of training objectives and these are specified in each example.

The mathematical models presented are made up of ordinary differential and algebraic equations. Distributed systems such as heat exchangers are represented by a series of lumped parameter approximations. This fairly simple modelling approach is sufficient as long as the model allows the training objectives to be achieved. The majority of the programs also include fault diagnostic exercises. These are created by locally rewriting the model to simulate the process at that point, or by redefining input variables, so that abnormal operation is simulated and the changes proceed through the simulation.

The trainee is able to operate the simulations from animated mimic plant control panels. He can change the setpoint of each controller and observe the response on the screen display. When he has become familiar with the operation of the particular system the trainee can then introduce a random fault or disturbance. He can investigate the nature of the induced fault by changing setpoints and observing the response. Once he has diagnosed the fault the program will compare his diagnosis with the correct answer and give him feedback on his assessment. In this way the trainee can make decisions, carry out operating tasks and diagnose faults etc, and so learn about the operation of the system by discovery.

A detailed description of the simulation of 'Steam-heated Heat Exchanger Control' is given in the next section 7.2. The other examples of generic simulations are described briefly in the following sections. The usefulness of the programs was evaluated by obtaining the opinions of plant personnel. These opinions are presented in the discussion in section 7.6.

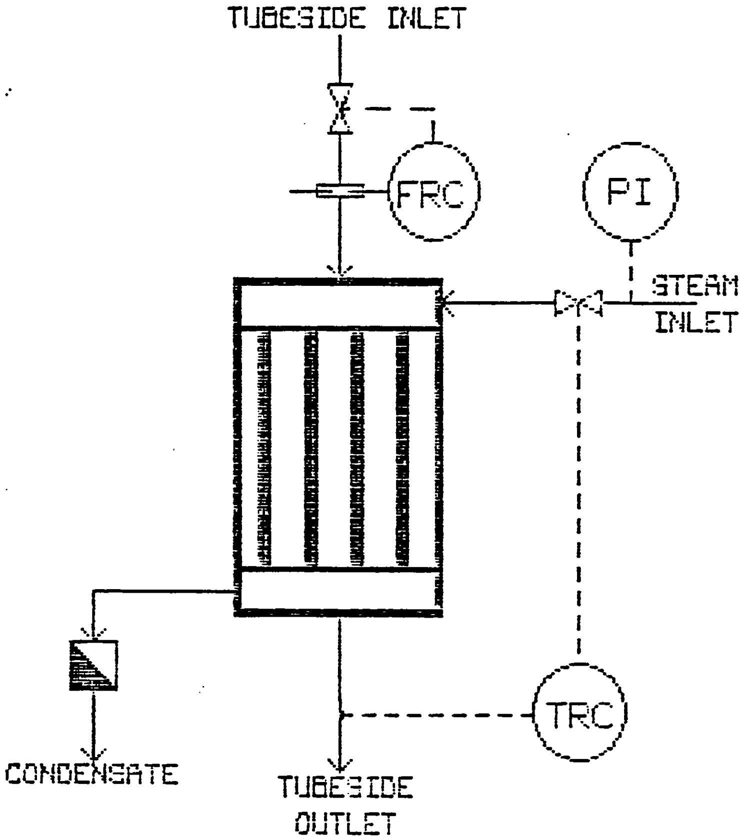
7.2 Heat Exchanger Control

7.2.1 Steam-Heated Heat Exchanger Control

7.2.1.1 Introduction

This program simulates the operation of the steam-heated heat exchanger control system shown in Figure 7.1.

Figure 7.1 : Steam-Heated Heat Exchanger Control System



It consists of a shell-and-tube heat exchanger where saturated steam condensing in the shell heats the cold fluid flowing through the tubes. The tubeside liquid flowrate is controlled at the inlet by a proportional + integral action controller, FRC, which opens and closes a control valve accordingly. The tubeside exit temperature is controlled by a proportional + integral + derivative action controller, TRC which varies the steam fed to the shell. The steam pressure in the shell is also displayed.

The program consists of two parts :-

(a) Simulation of operation

(b) Simulation of faults and disturbances and fault diagnosis.

Each part has some introductory instruction before the trainee is allowed to 'play' with the simulation to learn about the operation of the system by discovery.

The objectives of the simulation are :-

(a) To demonstrate the use of heat transfer in process operations.

(b) To demonstrate the operation of a steam-heated heat exchanger.

(c) To demonstrate the inherent slowness of temperature control.

(d) To demonstrate the effect of some common process faults and disturbances on a steam-heated heat exchanger.

(e) To demonstrate the effect of some common instrumentation faults on process operations.

(f) To give practice in fault diagnosis.

The structure of each part of the program is as given in Figure 6.1. The 'USE' language code for the lessons 'hxmod5' and 'hxmod5a' which make up the steam-heated heat exchanger program is given in Appendix 3.1. A description of the program as seen by the trainee is given in section 7.2.1.4. The modelling of the various faults and failures will be described later in section 7.2.1.3 but first of all a description of the equations which model the operation of the system will be described in the next section 7.2.1.2.

7.2.1.2 Mathematical Model

A detailed mathematical model of a heat exchanger involves the derivation of a set of partial differential equations to take account of the spatial variations of the parameters within the exchanger. However, a highly simplified model which shows the essential responses of the exchanger to changes in feed conditions and steam pressure is sufficient to achieve the objectives of the desired training.

Therefore, the exchanger can be respresented by a lumped parameter approximation. This takes the form of a continuously stirred tank surrounded by a steam jacket as shown in Figure 7.2. If the exchanger is large then the dynamics of the shellside can be ignored(R9).

Considering the tubeside, an ordinary differential equation can be written to describe the variation of the tubeside exit temperature, Tt2 with time, t due to changes in feed conditions and heat transfer rate :-

$$\rho t * Vt * Cp * \frac{dTt2}{dt} = ft1 * Cp * Tt1 + q - ft2 * Cp * Tt2 \qquad \text{........(7.1)}$$

where ρt = tubeside liquid density

Vt = tubeside volume

Cp = tubeside liquid specific heat capacity

Tt1 = tubeside liquid inlet temperature

Tt2 = tubeside liquid exit temperature

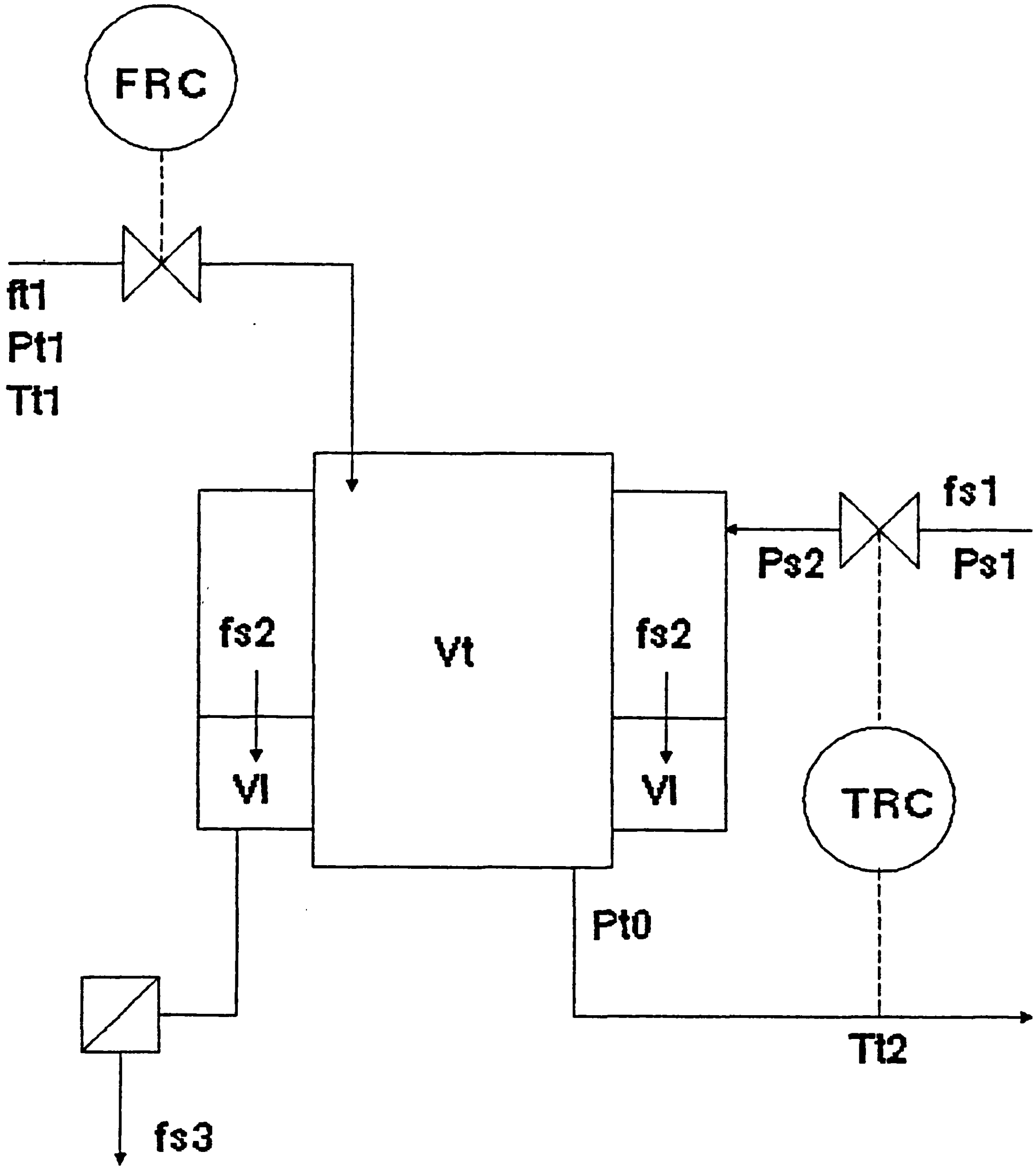
ft1 = tubeside liquid inlet flowrate

ft2 = tubeside liquid exit flowrate

q = overall heat transfer rate

The tubeside liquid specific heat capacity, Cp and density, ρt are assumed to be constant throughout the exchanger.

Figure 7.2 : Stirred Tank with Steam Jacket



The heat transfer rate, q between the shellside and tubeside is determined as follows assuming that the heat capacity of the barrier between the two sides is negligible :-

$$q = U * A * deltaT \qquad ....(7.2)$$

where U = overall heat transfer coefficient

A = heat transfer area

deltaT = log mean temperature difference

The available heat transfer area varies with the amount of condensate hold-up in the exchanger and therefore, assuming the tubes are arranged vertically :-

$$A = \frac{(Vstot - Vl) * Atot}{Vstot} \qquad ....(7.3)$$

where Vstot = total shellside volume

Vl = shellside condensate hold-up

Atot = total heat transfer area

The temperature difference, deltaT is calculated from :-

$$deltaT = \frac{(Ts - Tt1) - (Ts - Tt2)}{\ln((Ts - Tt1)/(Ts - Tt2))} \qquad ....(7.4)$$

where Ts = shellside steam temperature

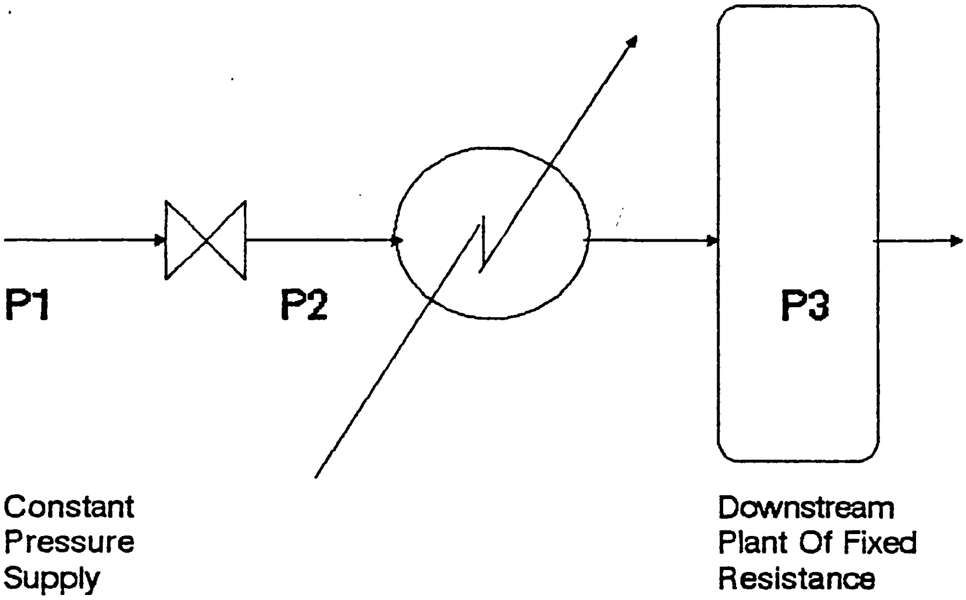
The quantity (Ts - Tt1)/(Ts - Tt2) is monitored to ensure that it does not become greater than 10^{15} or less than 10^{-13} as this causes the number range of the Regency microcomputer to be exceeded. This can occur as the tubeside exit temperature approachs the shellside steam temperature and also if there is a sudden increase in the tubeside liquid inlet flowrate. In such situations, the quantity is set to the maximum or minimum value possible.

The tubeside liquid flowrate is calculated by considering the pressure drop over both the exchanger and the upstream flow control valve. Consider the arrangement shown in Figure 7.3. For a constant flow F, the liquid flow through the control valve is given by :-

$$F = Cv\sqrt{(P1 - P2)} \qquad \qquad ....(7.5)$$

where Cv = valve discharge coefficient

Figure 7.3 : Pressure Drop Calculation



Assuming that the flow through the exchanger is also proportional to the square root of the pressure drop then the flow, F is also given by :-

$$F = K\sqrt{(P2 - P3)} \qquad \text{........(7.6)}$$

where K = constant

Combining these two equations to eliminate the intermediate pressure, P_2 gives :-

$$F = Cv * \sqrt{\frac{(P1 - P3)}{(1 + K * Cv * Cv)}} \qquad \text{........(7.7)}$$

Rewriting this equation enables the tubeside liquid inlet flowrate, ft1 to be calculated from :-

$$ft1 = ftCv * \sqrt{\frac{(Pt1 - Pt2)}{(1 + K * ftCv * ftCv)}} \qquad \text{........(7.8)}$$

where ftCv = tubeside liquid flow control valve coefficient

Pt1 = tubeside liquid flow supply pressure

Pt2 = tubeside liquid flow exit pressure

The tubeside exit flowrate, ft2 can then be calculated from :-

$$ft2 = ft1 \qquad \text{........(7.9)}$$

The steam condensation rate, fs2 is dependent on the amount of heat transfer and therefore it can be calculated from :-

$$fs2 = \frac{q}{\triangle Hvap} \qquad \text{.......(7.10)}$$

where $\triangle$Hvap = latent heat of vaporisation

The steam feedrate, fs1 can then be calculated assuming that total condensation occurs :-

$$fs1 = fs2 \qquad ....(7.11)$$

The steam feedrate can also be calculated from the flow through the shellside flow control valve :-

$$fs1 = fsCv * \sqrt{\frac{(Ps1 - Ps2)}{\rho s}} \qquad ....(7.12)$$

where fsCv = shellside vapour flow control valve coefficient

Ps1 = steam supply pressure

Ps2 = shellside steam pressure

ρs = saturated steam density

By combining the two equations, the shellside steam pressure, Ps2 for given control valve position can be determined. The steam in the shell is assumed to be saturated and therefore the steam temperature, Ts corresponding to a saturation pressure of Ps2 can be determined from data. This new temperature can then be used in the next solution of the model equations.

The condensate flow out of the exchanger through the steam trap, fs3 can be determined from :-

$$fs3 = stCv * \sqrt{Ps2 + \frac{(Vl * \rho l * g)}{Axsect} - Ps3} \qquad ....(7.13)$$

where stCv = steam trap discharge coefficent

ρl = condensate density

Ps3 = condensate discharge pressure

Axsect = Cross sectional area of exchanger

The volume of condensate hold-up, Vl in the exchanger can be obtained from an ordinary differential equation :-

$$\frac{dVl}{dt} = fs2 - fs3 \qquad ....(7.14)$$

This value can then be used in the next solution of the equations to determine the available heat transfer area. However there should be no condensate hold-up in the exchanger if the steam trap is working correctly.

These equations can then be solved using the algorithm shown in Figure 6.2 and described in section 6.4.2. Equations 7.2, 7.3, 7.4, 7.8, 7.9, 7.10, 7.11, 7.12 and 7.13 are the algebraic equations. Equations 7.1 and 7.14 contain the time dependent derivatives. The integration is carried out using the 'intin' and 'intde' routines described in Appendix 2.

The tubeside inlet flow control loop is modelled using the 'PIcontr' routine. The tubeside exit temperature controller is modelled using the 'PIDcontr' routine. The discharge coefficients of the two control valves are modelled using the 'valve' routine. These routines are also described in Appendix 2. The 'USE' language code for the simulation calculations are given in section 'simcalcs' of the lesson 'hxmod5a' in Appendix 3.1.

7.2.1.3 Fault Simulation

The program includes 12 process faults and disturbances and 8 instrument faults and failures. These are listed in Table 7.1. The faults are simulated by 'switching' various parts of the mathematical model on and off and by changing the values of some parameters. The 'switching' and changes are carried out by the routine 'fault' of the 'USE' lesson 'hxmod5a' given in Appendix 3.1 to simulate the particular random fault selected.

Referring to Table 7.1, fault no's 1 and 2 are achieved by 'switching off' the modelling of the tubeside inlet flow control valve. In the case of fault 1 this gives the effect of the valve jamming in its current position and in the case of fault 2, the discharge coefficient is calculated to its maximum value to give the effect of the valve failing open. Fault no's 3 and 4 for the steam flow control valve are achieved in a similar fashion. Fault 5 is achieved by 'switching off' the modelling of the steam trap outlet flow to give the effect of the steam trap failing.

Fault no's 6 and 7 are achieved by making step changes in the calculated value of the tubeside inlet flowrate, ft1. Similarly, fault no's 8 and 9, and, 11 and 12 are achieved by making step changes in the tubeside inlet flow supply pressure, Pt1 and the steam supply pressure, Ps1. Fault 10 is achieved by decreasing the overall heat transfer coefficient, U to give the effect of the exchanger becoming fouled.

Table 7.1 Steam-Heated Heat Exchanger Control Process and Instrument Faults, Disturbances and Failures.

Process Faults And Disturbances

1. Tubeside inlet flow control valve jammed

2. Tubeside inlet flow control valve failed open

3. Steam flow control valve jammed

4. Steam flow control valve failed open

5. Steam trap failed

6. Surge in tubeside inlet flowrate

7. Drop in tubeside inlet flowrate

8. Increase in tubeside flow supply pressure

9. Decrease in tubeside flow supply pressure

10. Fouling of exchanger

11. Increase in steam supply pressure

12. Decrease in steam supply pressure

Instrument Faults and Failures

13. Total instrument air failure

14. Tubeside inlet flowrate chart recorder pen stuck

15. Tubeside exit temperature chart recorder pen stuck

16. Tubeside inlet flowrate chart recorder inlet air failure

17. Tubeside exit temperature chart recorder inlet air failure

18. Tubeside inlet flowrate controller air failure

19. Tubeside exit temperature controller air failure

20. Steam pressure indicator air failure

Fault 13 is achieved by 'switching off' the modelling of both the process controllers and the updating of the chart recorder displays and the steam pressure indicator. The flow control valve discharge coefficients are also calculated to their 'fail-safe' positions of fully open for the tubeside flow and shut for the steam flow.

Fault no's 14 and 15 are simulated by 'switching off' the respective part of the routine 'chartdat' which models the updating of the information displayed on the chart recorders.

Fault no's 16 and 17 are simulated by 'switching off' the modelling of the respective process controller and calculating the controller output signal to the maximum possible to produce the effect of a loss in input air signal to the controller. In addition, the respective part of the routine 'chartdat' would be 'switched off' since the loss of input air signal would also result in no change in the displayed chart recorder information.

Fault no's 18 and 19 are simulated by 'switching off' the respective process controller together with the respective part of routine 'chartdat'. In addition the respective flow control valve discharge coefficient is also calculated to it's 'failsafe' value to give the effect of a loss of instrument air to a particular controller.

Finally, fault no 20 is simulated by 'switching off' the routine 'pigauge' which models the steam pressure indicator.

An example of both a process and an instrumentation fault will be given in the program description which follows in the next section 7.2.4.

7.2.1.4 The Program as Seen by the Trainee

A sample of the screen displays seen by the trainee are given in Figures 7.4 to 7.15. Figures 7.4, 7.5, 7.6 and 7.7 introduce the trainee to the program. They describe aspects of the control system(e.g. Figure 7.5) and test the trainee's comprehension of the material presented(e.g. Figure 7.6). The mimic control panel display which will be used to operate the simulation is then described(e.g. Figure 7.7). It consists of two strip-chart process recorder-controllers, one for the tubeside inlet flowrate and one for the tubeside exit temperature. The controller signals to the respective control valves are shown as percentages above each chart recorder. The measured variables of flowrate and temperature are plotted on the charts and the setpoint of each controller is displayed in a box beneath each chart recorder. The steam supply pressure is also shown on a gauge at the top of the screen and a process flow diagram is shown beneath this for reference.

The trainee is then presented with an example setpoint change in tubeside inlet flowrate. The effect of the change is described such as in Figure 7.8. The trainee is then allowed to 'play' with the simulation at his own pace.

Figure 7.4 : Steam-Heated Heat Exchanger Control Title Screen

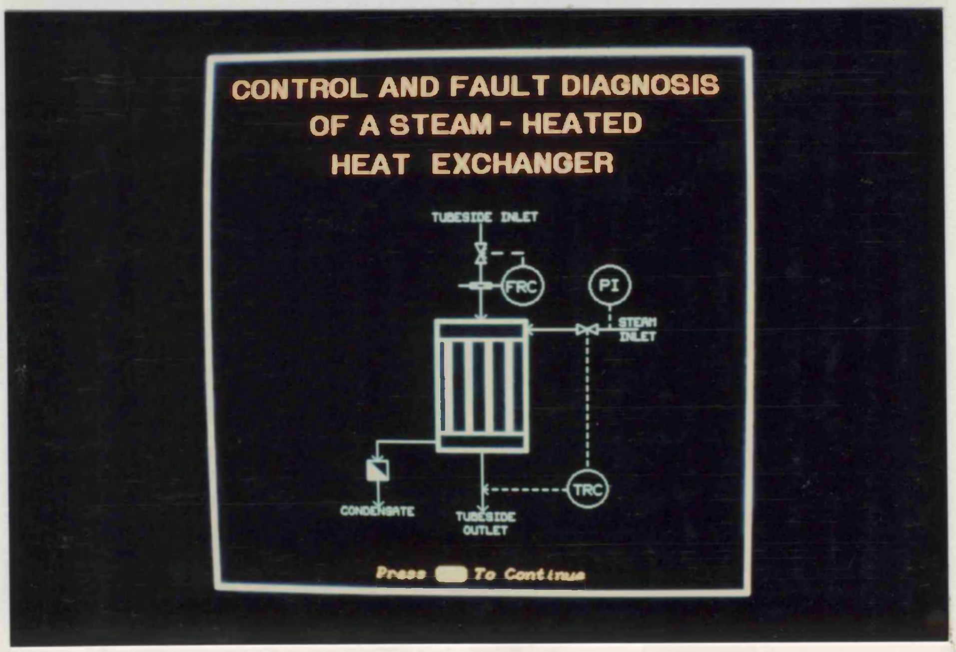


Figure 7.5 : Steam-Heated Heat Exchanger Control Introduction

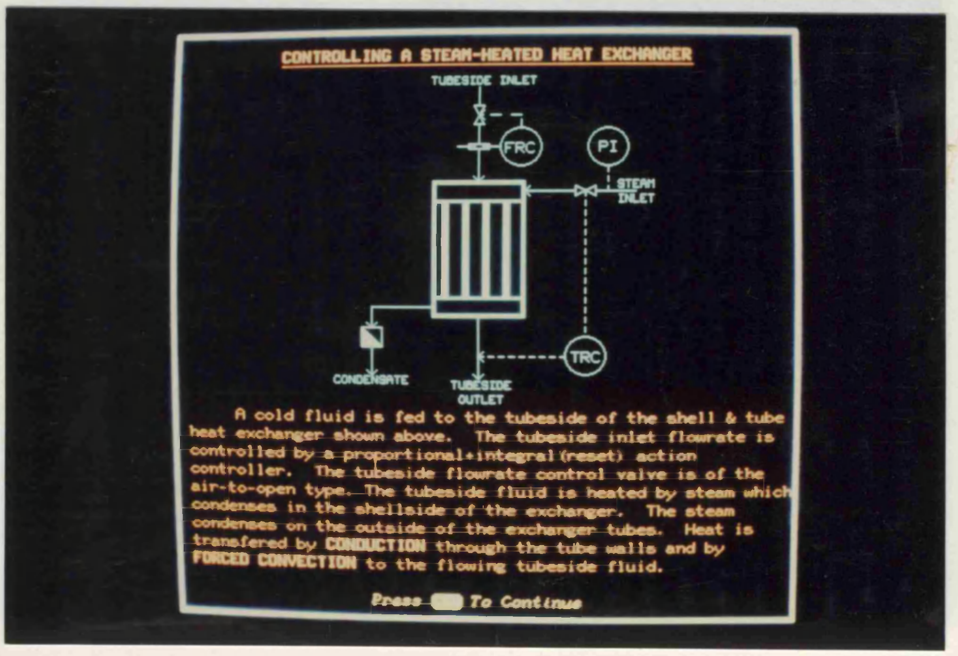


Figure 7.6 : Steam-Heated Heat Exchanger Control Test

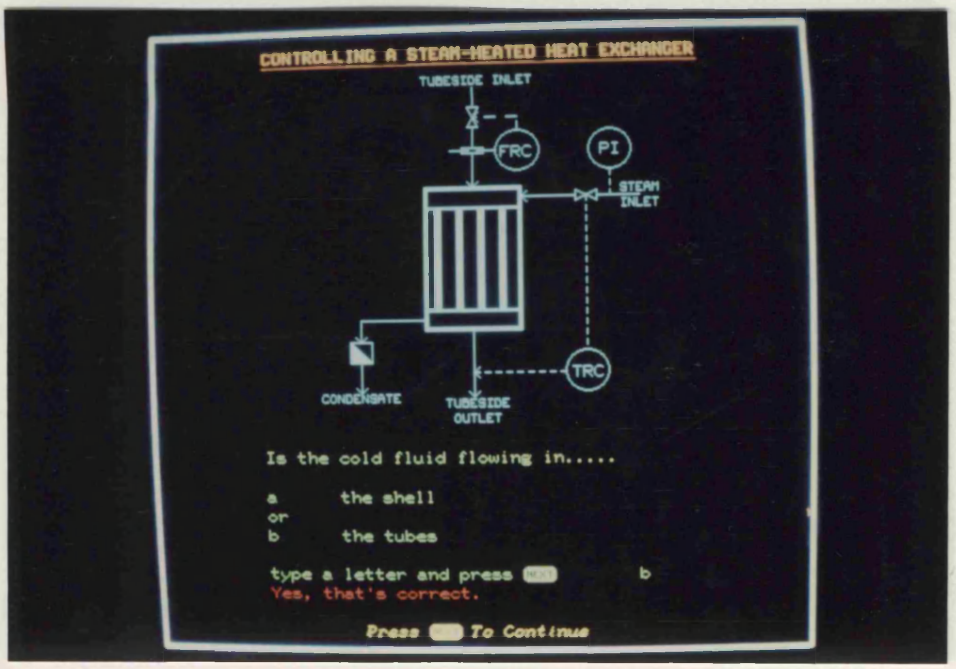


Figure 7.7 : Steam-Heated Heat Exchanger Control Mimic Plant Control Panel

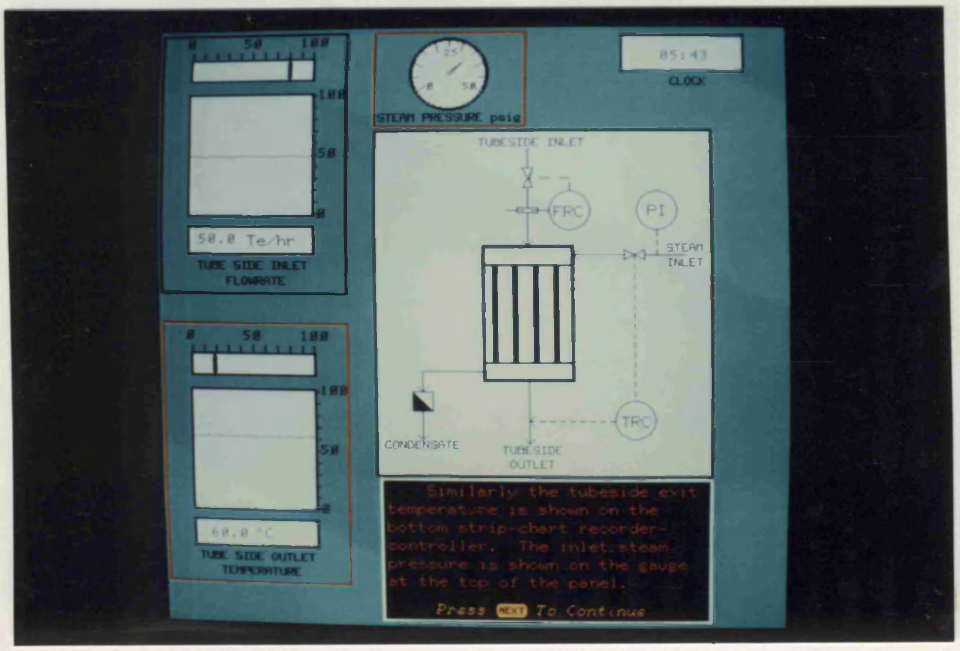


Figure 7.6 : Steam-Heated Heat Exchanger Control Test

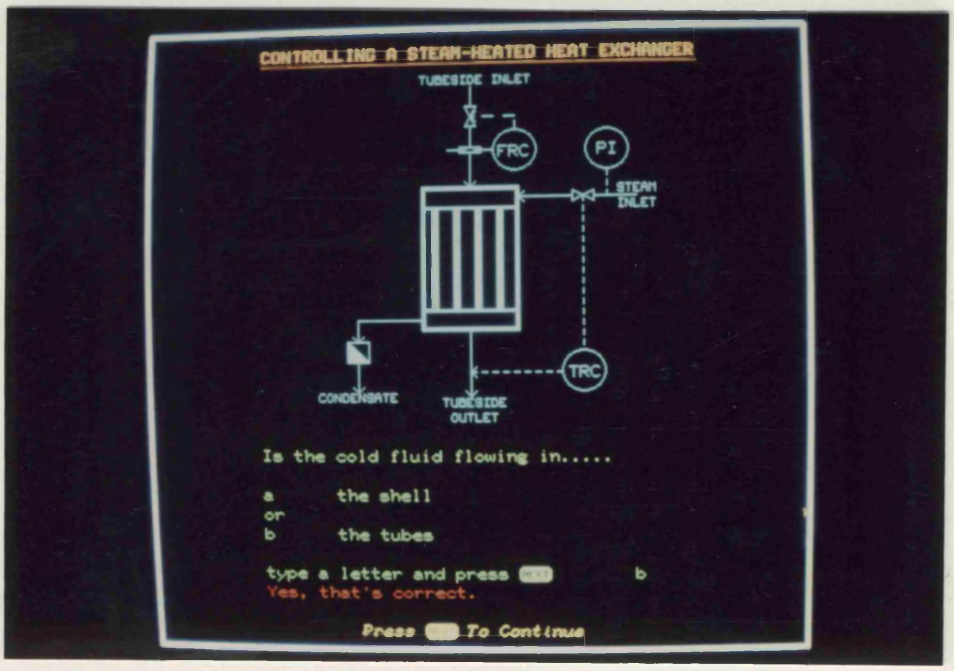


Figure 7.7 : Steam-Heated Heat Exchanger Control Mimic Plant Control Panel

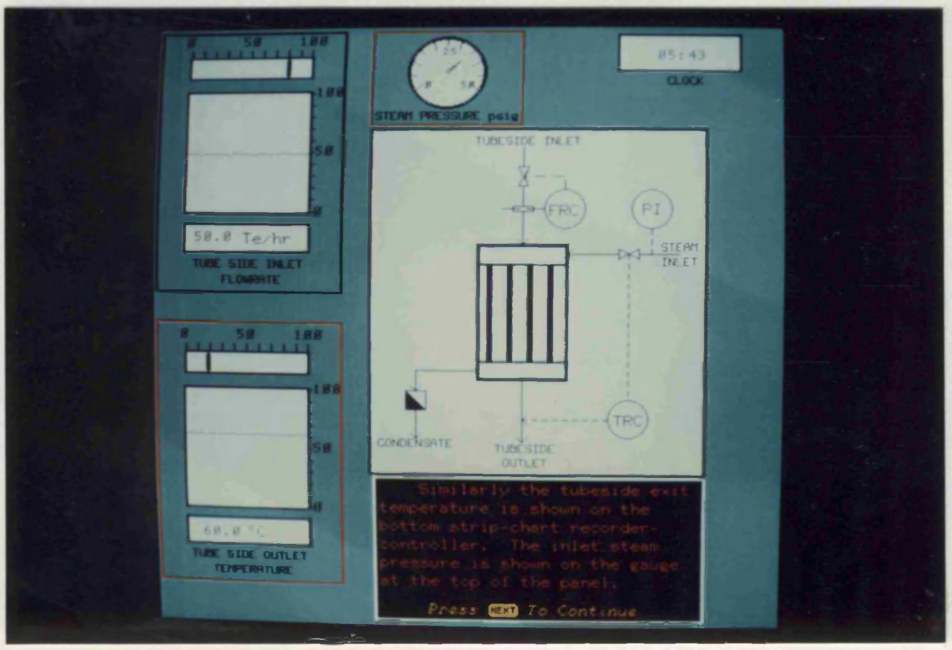


Figure 7.8 : Steam-Heated Heat Exchanger Control Setpoint Change

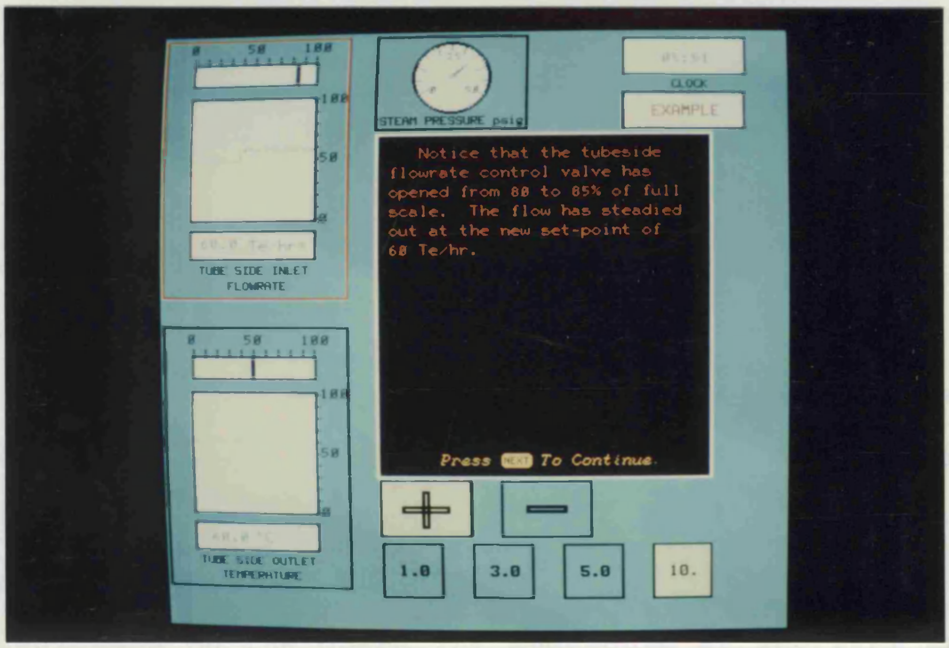
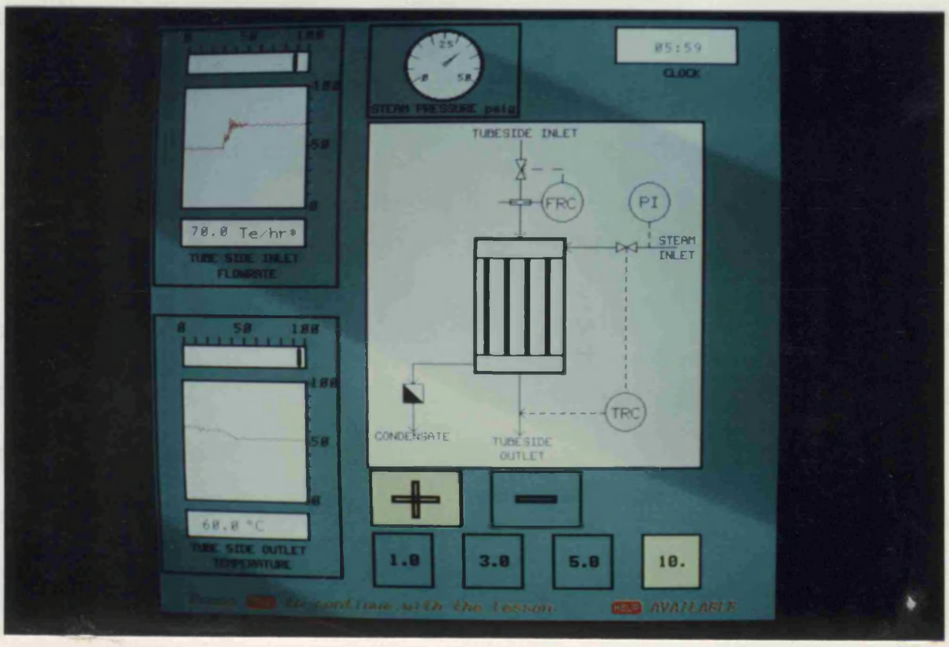


Figure 7.9 : Steam-Heated Heat Exchanger Control Simulation



A series of touch panel boxes are displayed on the screen as shown in Figure 7.9. In order to change the setpoint of one of the controllers, the trainee has to first of all select the direction of the change by touching the box marked '+' for up or '-' for down. Then, the magnitude of the desired change is specified by touching either the '1.0', '3.0', '5.0' or '10.' boxes. The boxes which he has touched illuminate to indicate the change to be made. Finally to change the controller setpoint by the specified amount he has just to touch the particular controller he wishes to change. This attempts to replicate normal control room thought processes as described in section 6.3. The trainee can obtain guidance on the operating procedure at any time when the simulation is running by pressing the 'help' key. In this way, the trainee can investigate the response of the system to various setpoint changes and so learn about the system by discovery.

Once the trainee has become familiar with the operation of the system he can move on to the second section of the program on faults and fault diagnosis. The trainee is introduced to possible faults and methods of detecting them(e.g. Figure 7.10). He is then given an example process disturbance of a surge in inlet flowrate. The effect of the disturbance is described as in Figure 7.11. He is also given an example instrument fault of a sticking chart recorder pen and once again its effect is described as in Figure 7.12.

Figure 7.10 : Steam-Heated Heat Exchanger Control Fault Diagnosis Introduction

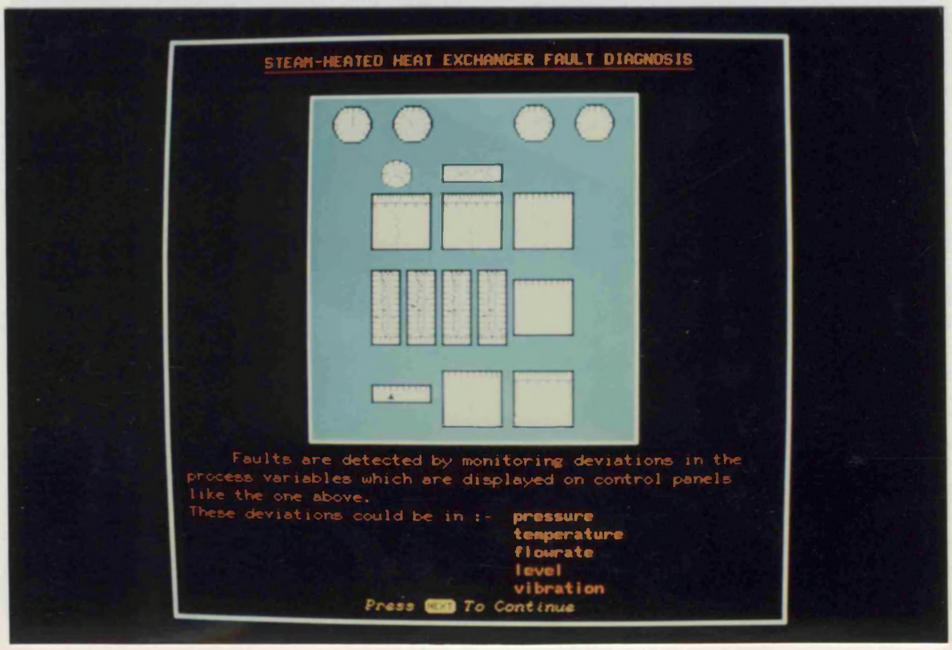


Figure 7.11 : Steam-Heated Heat Exchanger Control Fault Diagnosis Process Disturbance

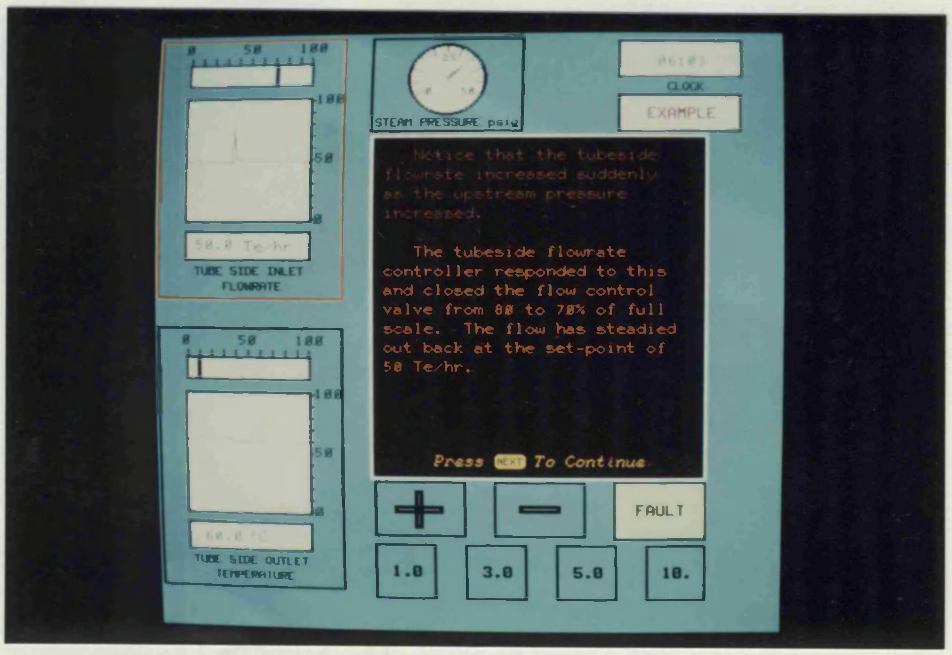


Figure 7.12 : Steam-Heated Heat Exchanger Control Fault Diagnosis
Instrument Fault

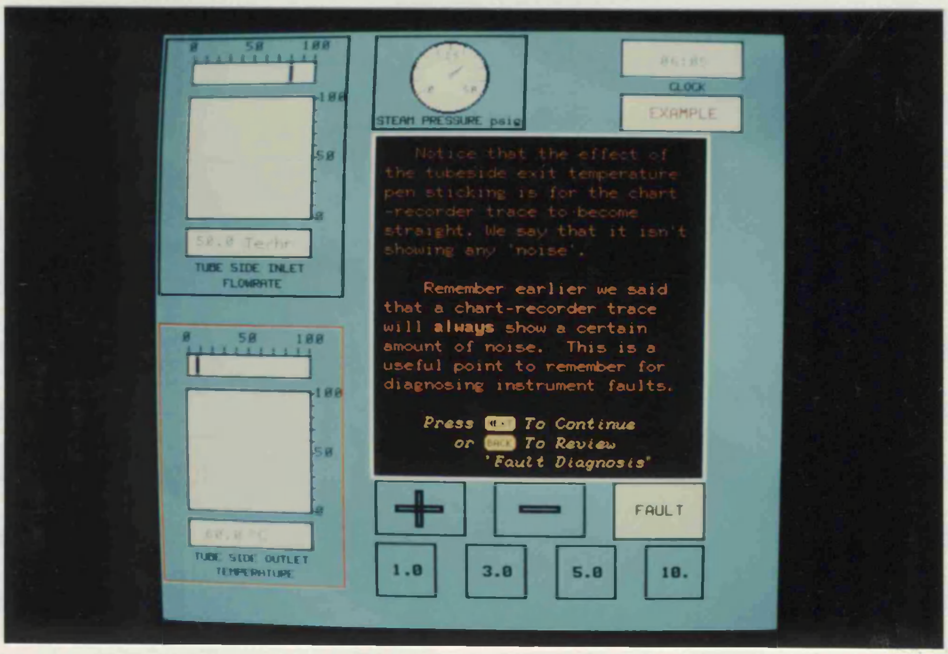
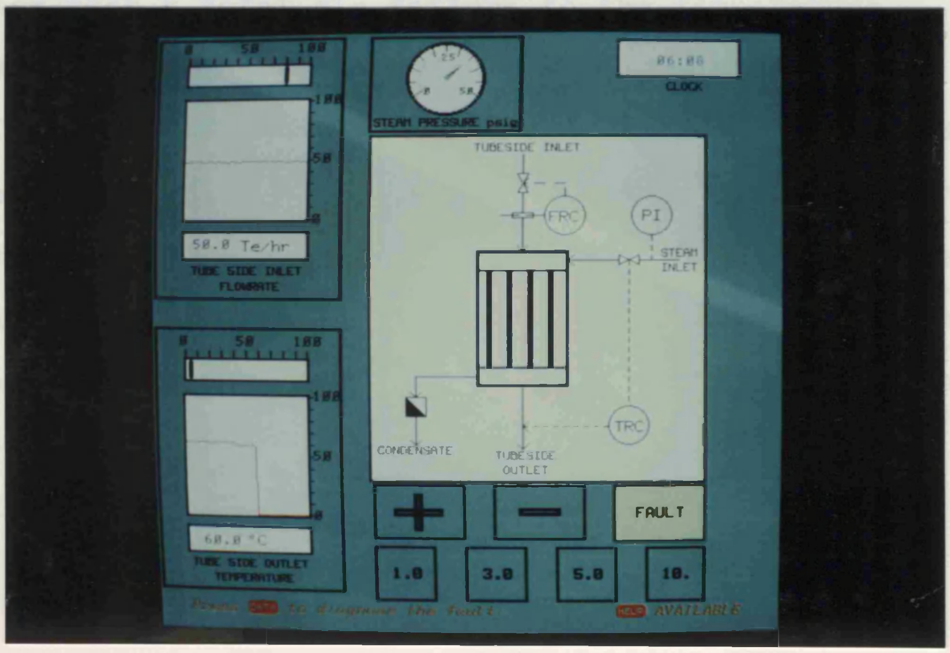


Figure 7.13 : Steam-Heated Heat Exchanger Control Fault Diagnosis
Fault Simulation



Finally the trainee is allowed to operate the system and introduce faults entirely at his own pace. The two example faults are included in the twenty faults which are selected at random by the program when the trainee touches the box marked 'FAULT'. A typical display with a fault introduced is shown in Figure 7.13. This particular fault is a failure in the tubeside exit temperature controller air supply. The trainee is asked to attempt to diagnose the nature of the induced fault and to switch to the 'fault diagnosis' display as shown in Figure 7.14 when he thinks he knows what it is. In this case the trainee has selected fault no 17 which is a loss in temperature controller input air sugnal. Since this fault is partly correct the program gives the trainee guiding feedback on where to look for information which will help in selecting the correct answer. It suggests that the trainee should look at the control valve position.

Figure 7.13 shows the valve position to be zero. This indicates that a total air failure to the temperature controller has occurred rather than just a loss of input air signal. Figure 7.15 confirms that the correct answer is in fact fault no 19. Once the trainee has diagnosed the fault correctly he can return to the simulation either at the same point at which he left but with the fault removed so that he can see the effect of removing the fault or to the normal steady-state conditions so that another fault can be introduced.

Figure 7.14 : Steam-Heated Heat Exchanger Control Fault Diagnosis
Incorrect Diagnosis

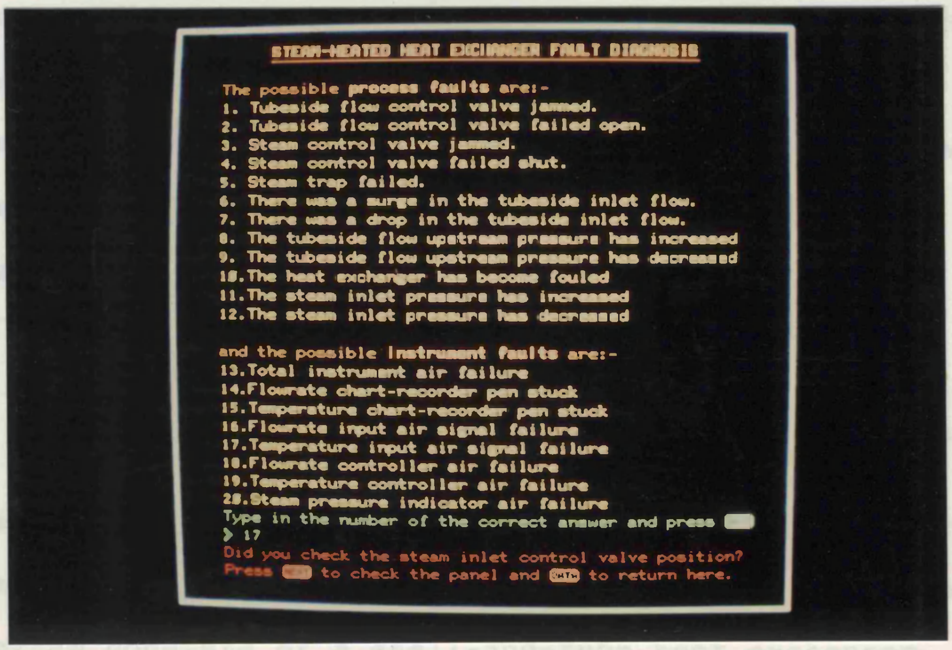
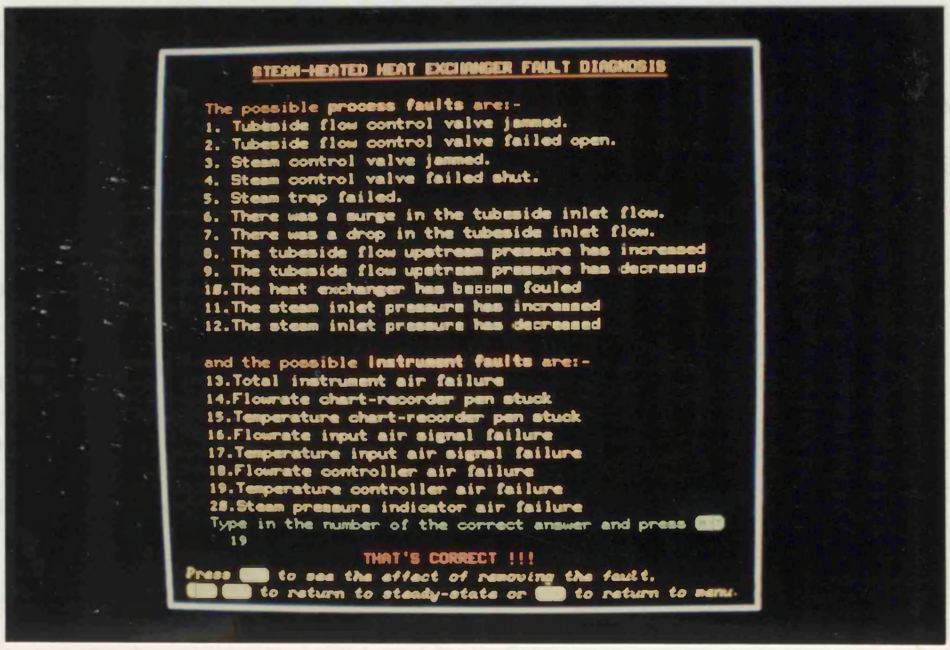


Figure 7.15 : Steam-Heated Heat Exchanger Control Fault Diagnosis
Correct Diagnosis



The trainee will discover that the fault diagnosis of the steam-heated heat exchanger requires careful observation of the control panel responses. The effects of the faults and disturbances are often masked initially by the inherent slowness of response of heat transfer controlled processes. Therefore, the simulation presents the trainee with a challenging learning situation.

7.2.2 Co-Current and Counter-Current Heat Exchanger Control

These two programs are similar to the one presented for Steam-Heated Heat Exchanger Control in the previous section. Each program consists of a shell-and-tube heat exchanger where the hot fluid flowing on the shellside heats the cold fluid flowing through the tubes. The tubeside fluid inlet flowrate is controlled by a proportional + integral action controller, FRC. The tubeside exit temperature is controlled by a proportional + integral + derivative action controller, TRC which varies the shellside fluid inlet flowrate accordingly. The shellside exit temperature is also monitored by a chart recorder, TR. The co-current heat exchanger control system is shown in Figure 7.16 and the counter-current arrangement in Figure 7.17.

The modelling of co-current and counter-current heat exchanger configurations requires that the spatial variations of the parameters within the exchanger are taken into account.

Figure 7.16 : Co-Current Heat Exchanger Control System

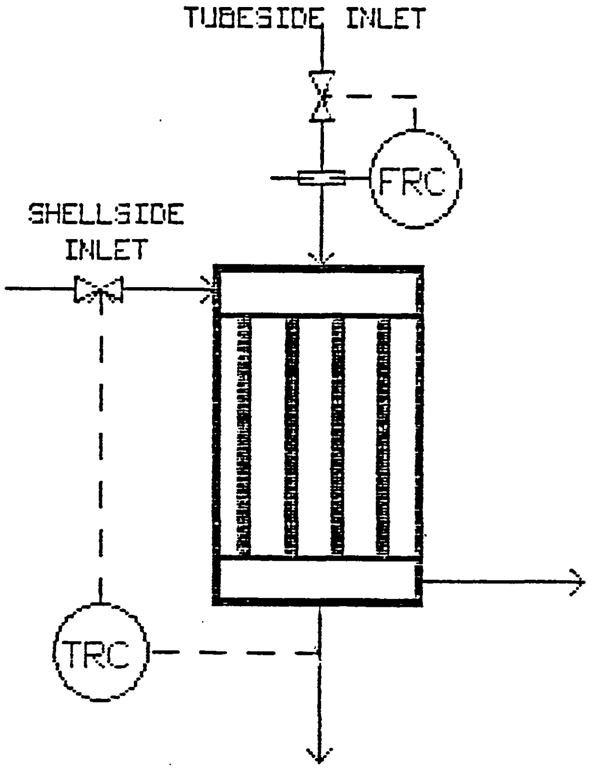
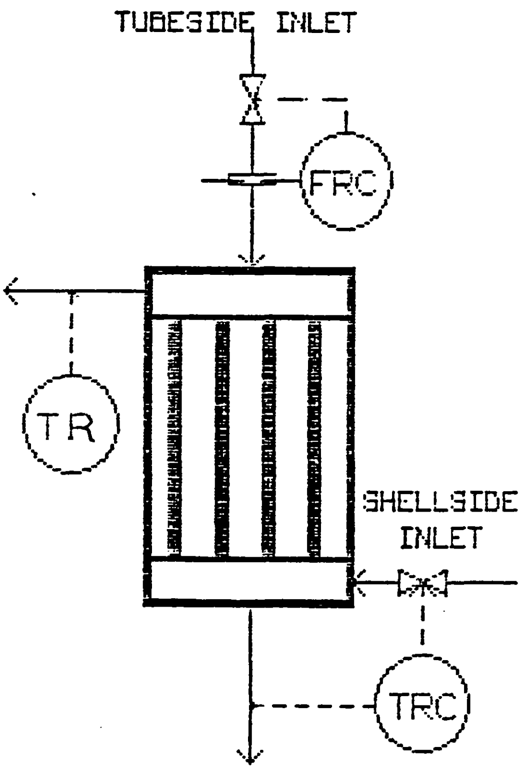


Figure 7.17 : Counter-Current Heat Exchanger Control System



The previous example, 'Steam-Heated Heat Exchanger Control' presented in section 7.2.1 was modelled using a simple lumped parameter approximation. This took the form of a continuously stirred tank surrounded by a steam jacket. In the case of the co-current and counter-current heat exchangers a series of lumped parameter approximations are required so that the model shows the essential responses of the exchanger to changes in tubeside and shellside feed conditions. Each lumped parameter approximation takes the form of a pair of continuously stirred tanks separated by a common heat transfer area as shown in Figure 7.18(C8).

The number of lumped parameter approximations used to model a particular heat exchanger depends on the dynamics of the exchanger. In these generic examples a couple of increments are sufficient to achieve the desired training objectives. However, if an actual plant exchanger is being modelled then enough increments have to be used to enable the actual plant dynamics to be sufficiently represented. This will be considered in the next chapter in section 8.3.

The programs each include 10 process faults and disturbances and these are listed in Table 7.2. The faults are simulated in a similar way to those described for the steam-heated heat exchanger in section 7.2.1.3.

Figure 7.18 : Pair of Stirred Tanks Model (C8)

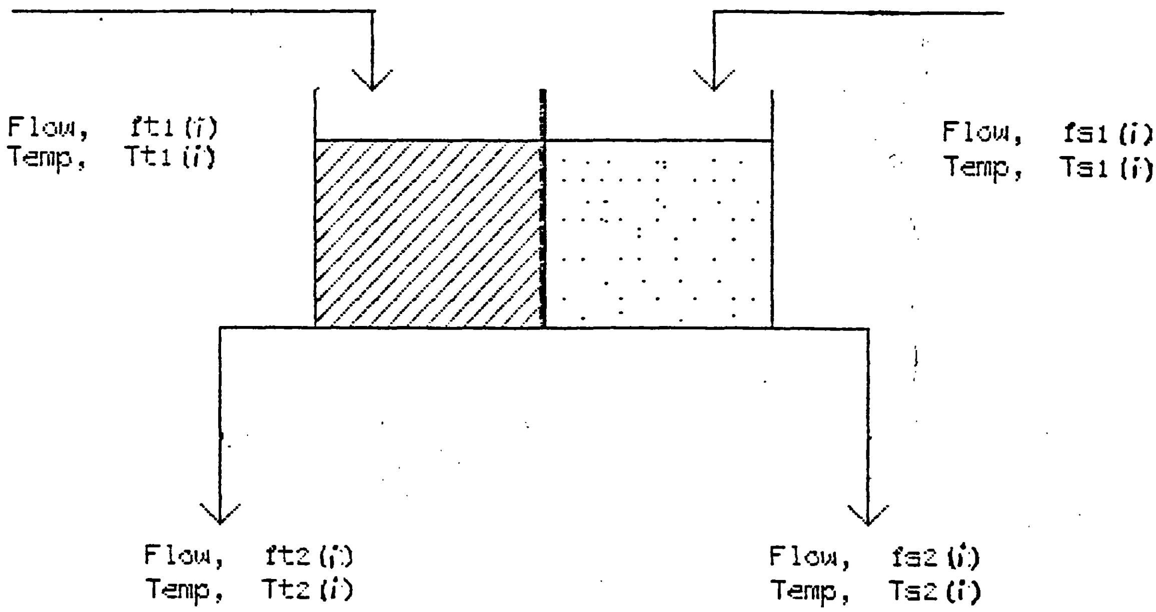


Table 7.2 Co-current and Counter-current Heat Exchanger Control Process Faults and Disturbances

Process Faults And Disturbances
1. Tubeside inlet flow control valve jammed
2. Tubeside inlet flow control valve failed open
3. Shellside inlet flow control valve jammed
4. Shellside inlet flow control valve failed shut
5. Surge in tubeside inlet flowrate
6. Drop in tubeside inlet flowrate
7. Increase in tubeside flow supply pressure
8. Decrease in tubeside flow supply pressure
9. Decrease in shellside flow supply pressure
10. Fouling of exchanger

A sample of the co-current and counter-current heat exchanger control program screen displays seen by the trainee are given in Figures 7.19 to 7.22. Figure 7.20 shows the effect of the tubeside inlet flow control valve failing open on the co-current heat exchanger. Figure 7.22 shows the counter-current heat exchanger at steady-state.

The 'USE' language code for the co-current heat exchanger program, 'hx1' is given in Appendix 3.3 and for the counter-current heat exchanger program, 'hx2' in Appendix 3.4.

Figure 7.19 : Co-Current Heat Exchanger Control Title Screen

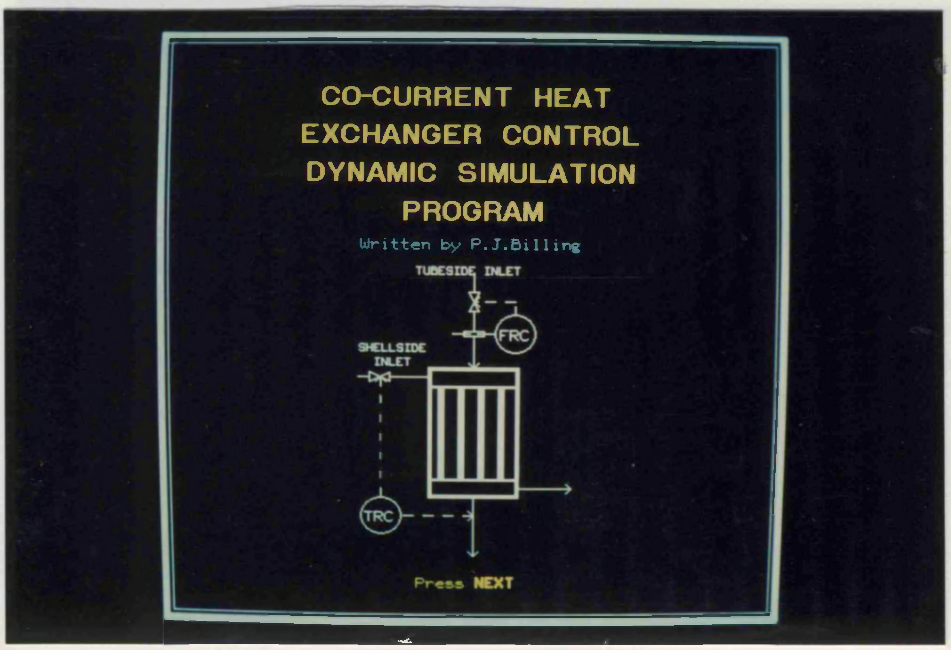


Figure 7.20 : Co-Current Heat Exchanger Control Mimic Plant Control Panel

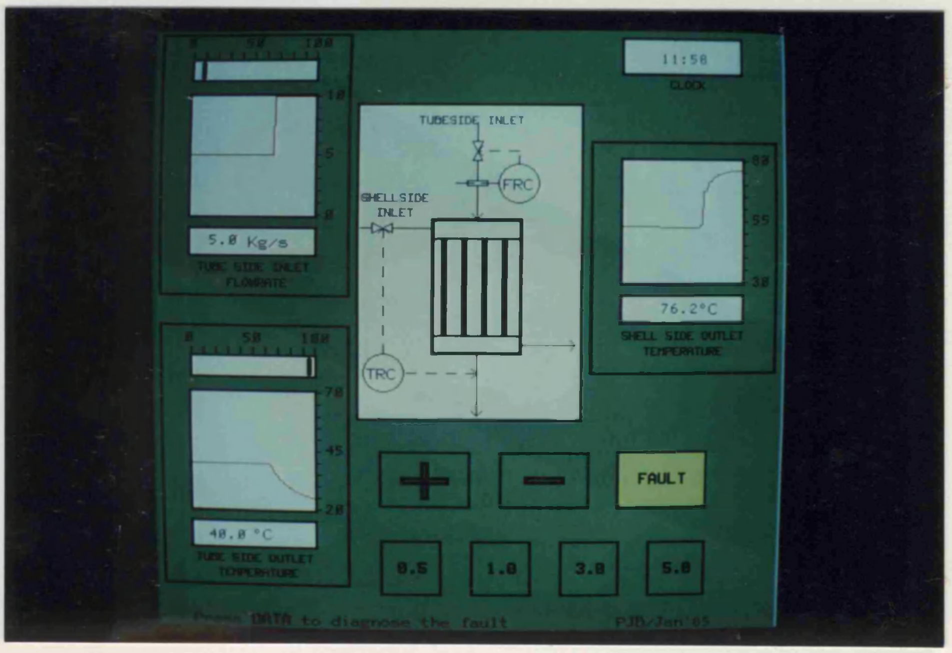


Figure 7.21 : Counter-Current Heat Exchanger Control Title Screen

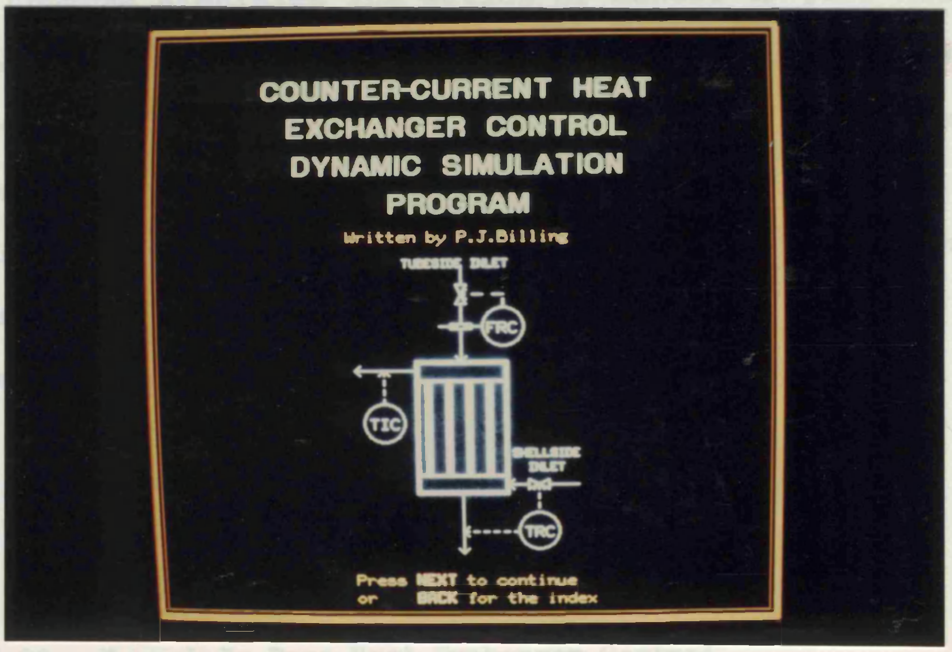
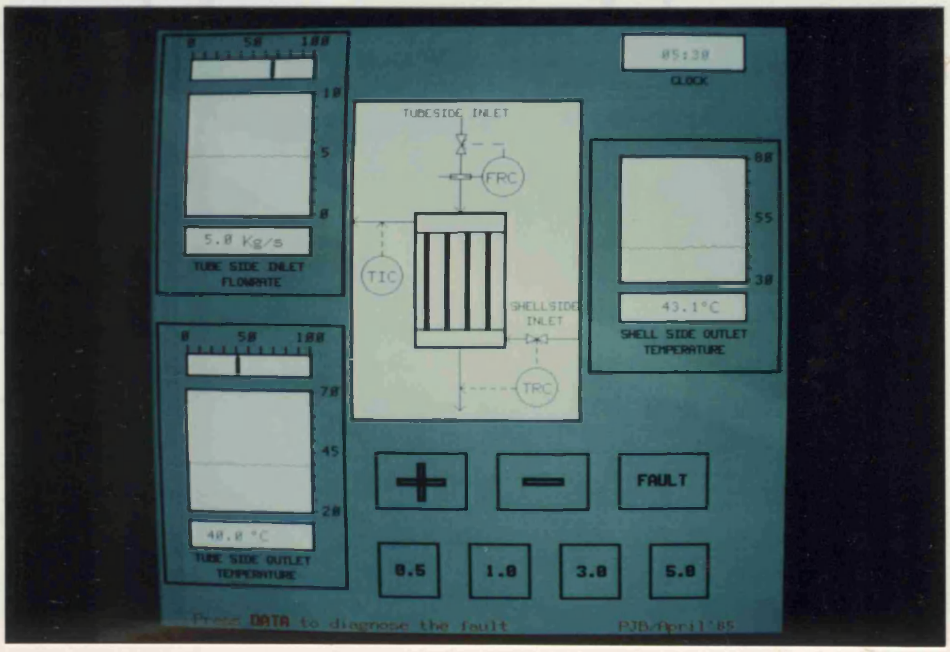


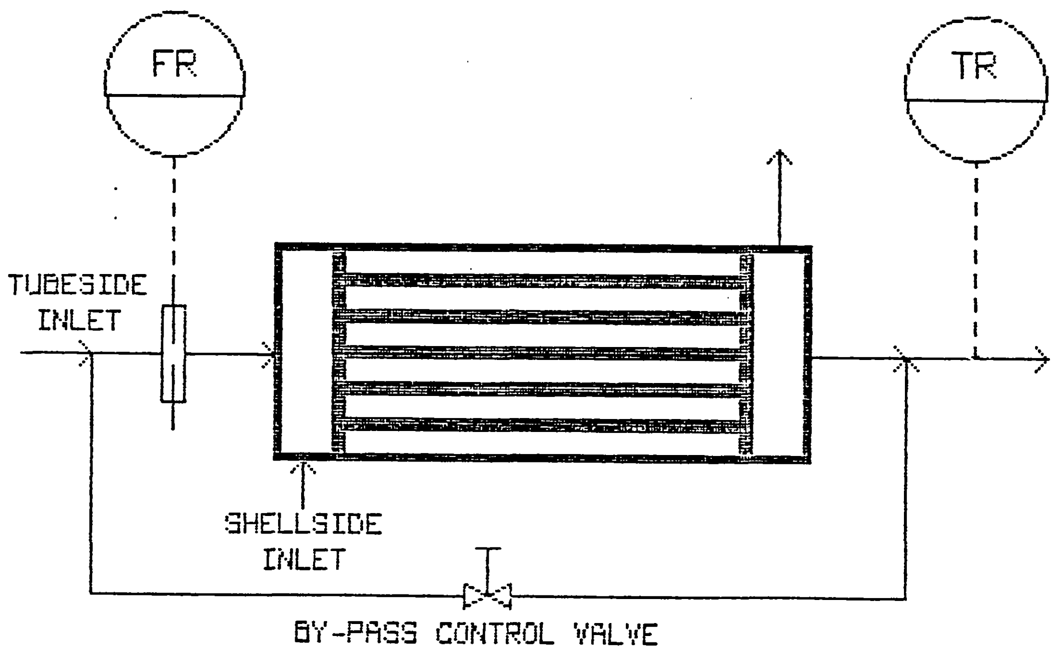
Figure 7.22 : Counter-Current Heat Exchanger Control Mimic Control Panel



7.2.3 Manual By-Pass Heat Exchanger Control

This program simulates the action of manual by-pass heat exchanger control system shown in Figure 7.23. It consists of a co-current heat exchanger where the control of the tubeside exit temperature is achieved by manually varying the flow of cold fluid by-passed around the exchanger. The tubeside inlet flowrate and exit temperature are monitored by recorders, FR and TR respectively.

Figure 7.23 : Manual By-Pass Heat Exchanger Control



The simulation was developed since process operators were finding it difficult to fully understand the effects of by-pass control. The program is presented in the form of a 'game' where the trainee is asked to control the output temperature at a set value by means of varying the by-pass valve. This is not as easy as it may seem!

A sample of the manual by-pass heat exchanger control program screen displays seen by the trainee are given in Figures 7.24 and 7.25. Figure 7.24 shows the opening display and the introduction which follows describes the control system, the operation of the simulation and the task of trying to control the tubeside exit temperature at 25C.

The control panel display given in figure 7.25 features two strip-chart recorders, one for the tubeside inlet flowrate and one for the tubeside exit temperature. Two touch panel option boxes are displayed in the centre of the screen and these allow the trainee to open and close the by-pass control valve as required.

The trainee will discover as shown in Figure 7.25 that controlling the temperature at 25C is not that easy. Opening the by-pass valve reduces the flow through the tubeside of the exchanger which in turn causes the temperature of the fluid exit the exchanger to rise. However, once the hot fluid from the exchanger is mixed with the cold by-pass flow the resulting temperature can show little change to what it was before the by-pass valved was opened.

Figure 7.24 : Manual By-Pass Heat Exchanger Control Title Screen

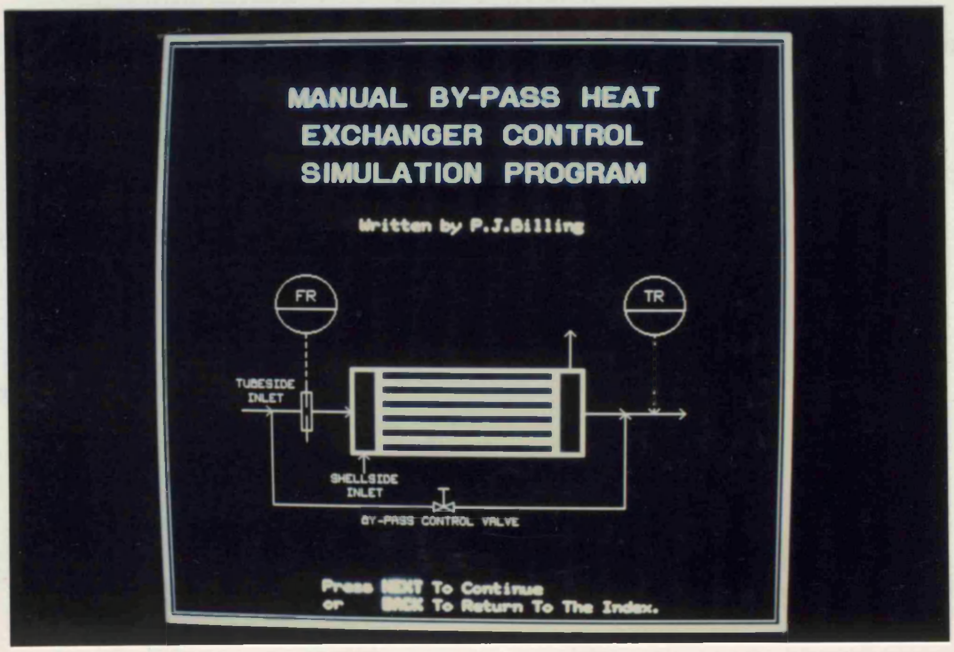
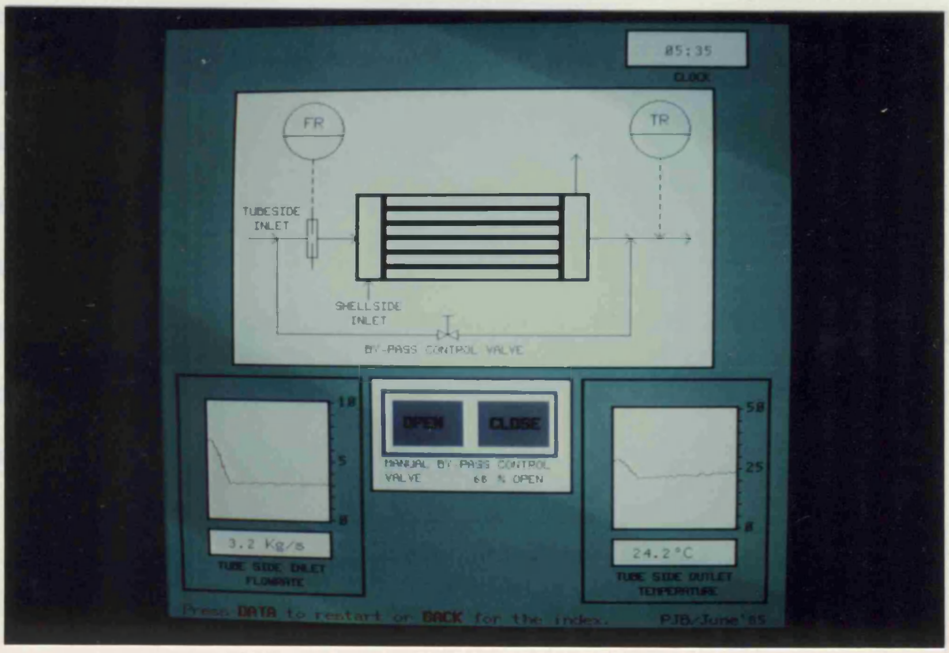


Figure 7.25 : Manual By-Pass Heat Exchanger Control Mimic Control Panel



Since there is a significant time lag between operating the by-pass valve and seeing the resultant exit temperature, careful, patient operation is required to maintain the exit temperature at the desired value.

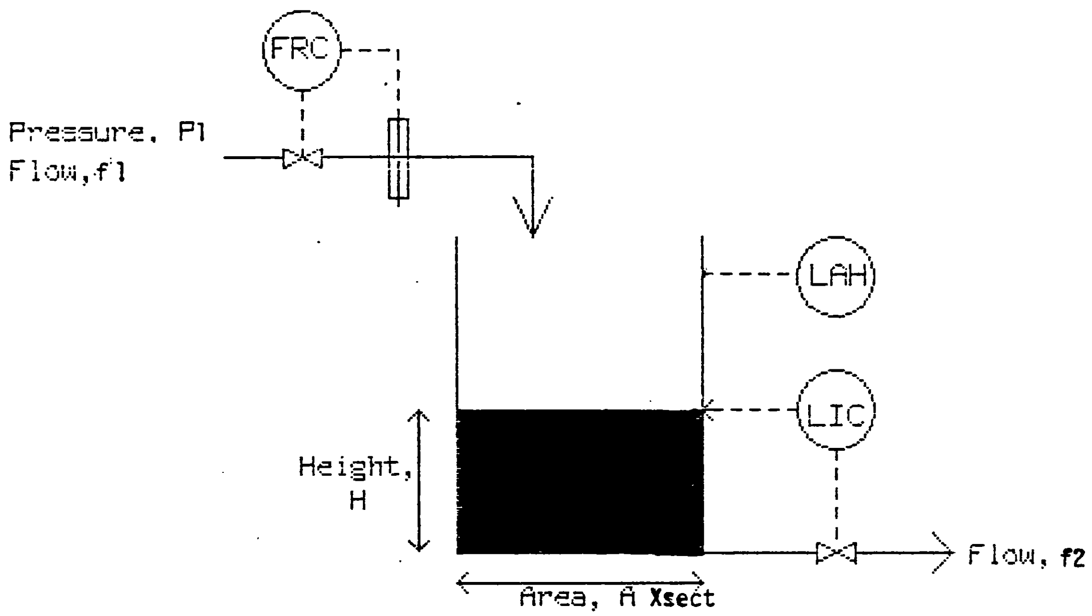
The 'USE' language code for the manual by-pass heat exchanger control program, 'hx3' is given in Appendix 3.5.

7.3 Tank Level Control

7.3.1 Introduction

This program simulates the action of a simple tank level control system as shown in Figure 7.26. It consists of a tank which is open to atmosphere and fed with a liquid at a flowrate, f1 and supply pressure P1. The liquid flowrate is controlled by a proportional + integral action controller, FRC, which opens and closes a control valve accordingly. The liquid level in the tank is controlled by a second proportional + integral action controller, LIC. This varies the exit flowrate from the tank, f2 by opening and closing a second control valve. A high level alarm is displayed when the level is above 90% of the tank's depth(B1).

Figure 7.26 : Tank Level Control System



The objectives of the simulation are :-

(a) To demonstrate the operation of a tank level control system.

(b) To give practice in the tuning of process controllers.

(c) To demonstrate the effect of some common process faults and disturbances on a tank level control system.

(d) To give practice in fault diagnosis.

The trainee is able to specify the settings for each of the two process controllers and is therefore able to go through the process of controller tuning.

The structure of the program is as given in Figure 6.1. The 'USE' language code for the tank level control program is given in lesson 'tk' in Appendix 3.2. A brief description of the program as seen by the trainee is given in section 7.3.3. First of all a description of the equations which model the system is given in the next section 7.3.2.

7.3.2 Mathematical Model

Considering the system shown in Figure 7.26, a mathematical model based on the one presented by Franks(F4) can be written to describe the operation of the tank level control system. An ordinary differential equation can be written to describe the variation of the height of liquid in the tank, H with time, t due to changes in the inlet flowrate, f1 and the exit flowrate, f2 assuming that the tank is well mixed :-

$$AXsect * \frac{dH}{dt} = f1 - f2 \qquad ....(7.15)$$

where AXsect = cross sectional area of the tank

The feed flowrate can be related to its supply pressure, P1 as follows :-

$$f1 = fCv\sqrt{P1} \qquad ....(7.16)$$

where fCv = inlet flow control valve discharge coefficient

This assumes that the pressure drop over the flowmeter and the control valve is comparable with the supply pressure, P1.

Similarly the exit flowrate, f2 can be related to the head of liquid in the tank, H :-

$$f2 = lCv \sqrt{H} \qquad \ldots\ldots\ldots(7.17)$$

where lCv = level control valve discharge coefficient

These equations can be solved using the algorithm shown in Figure 6.2 and described in section 6.4.2. Equations 7.16 and 7.17 are the algebraic equations and equation 7.15 is the time dependent derivative. The integration is carried out using the routines 'intin' and 'intde'. The inlet flow and tank level control loops are modelled using the 'PIcontr' routine. The discharge coefficients of the two control valves are modelled using the 'valve' routine. These routines are described in Appendix 2.

The program includes 8 process faults and disturbances and these are listed in Table 7.3. The faults are simulated in a similar way to those described for the steam-heated heat exchanger in section 7.2.1.3. The 'USE' language code for the simulation calculations are given in section 'simcalcs' and for the fault simulation in section 'fault' of the lesson 'tk' given in Appendix 3.2.

Table 7.3 Tank Level Control Process Faults and Disturbances.

Process Faults And Disturbances

1. Inlet flow control valve jammed
2. Inlet flow control valve failed shut
3. Tank level control valve jammed
4. Tank level control valve failed open
5. Surge in inlet flowrate
6. Drop in inlet flowrate
7. Increase in inlet flow supply pressure
8. Decrease in inlet flow supply pressure

7.3.3 The Program as Seen by the Trainee

A sample of the screen displays seen by the trainee are given in Figures 7.27 to 7.30. Figure 7.27 shows the opening display and the introduction which follows describes the control system and the operation of the simulation. The trainee is then asked to specify the settings for each of the process controllers as shown in Figure 7.28. The program then passes to the mimic control panel display shown in Figure 7.29.

The control panel display features a strip-chart recorder-controller for the inlet flowrate. The controller signal to the valve is shown as a percentage above the chart. The flowrate indication is plotted on the chart in terms of percentage of full scale.

Figure 7.27 : Tank Level Control Title Screen

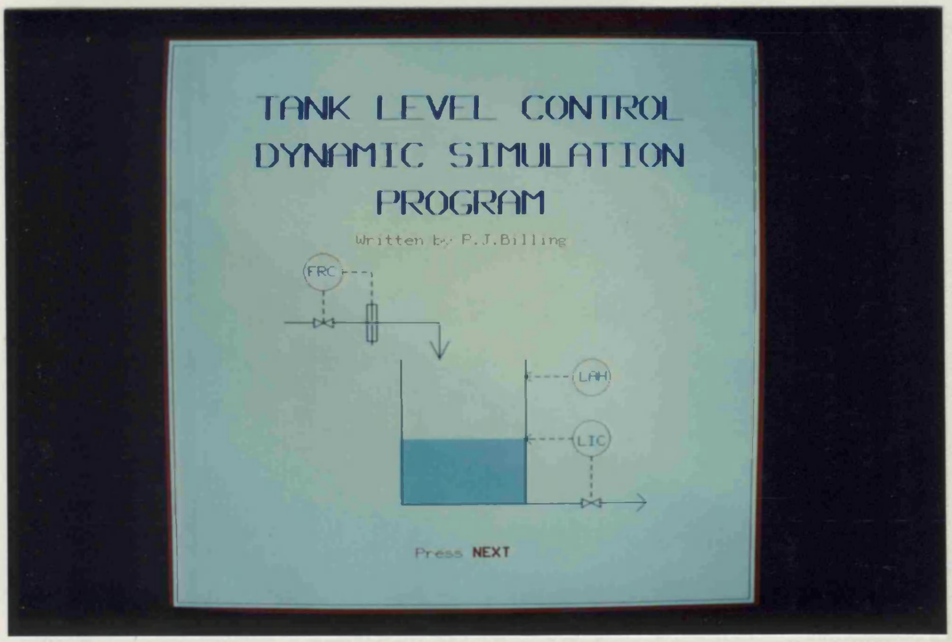


Figure 7.28 : Tank Level Control Controller Setting

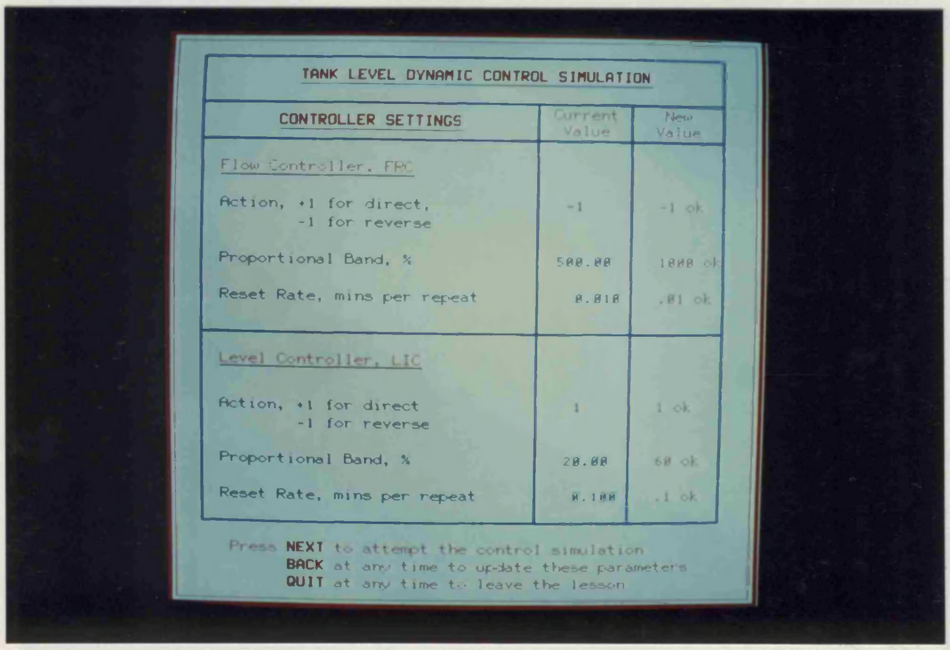


Figure 7.29 : Tank Level Control Mimic Plant Control Panel

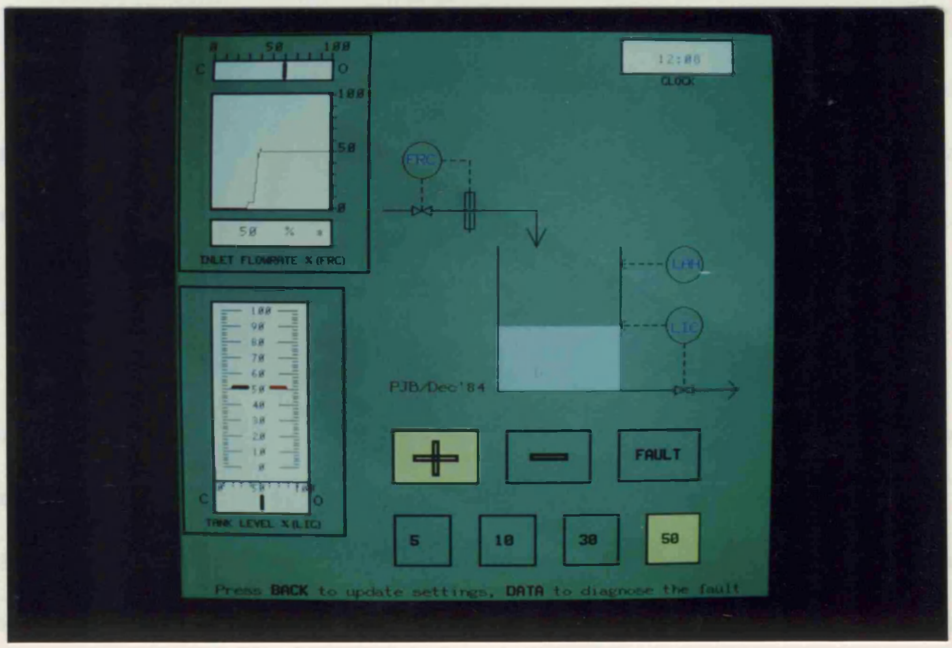
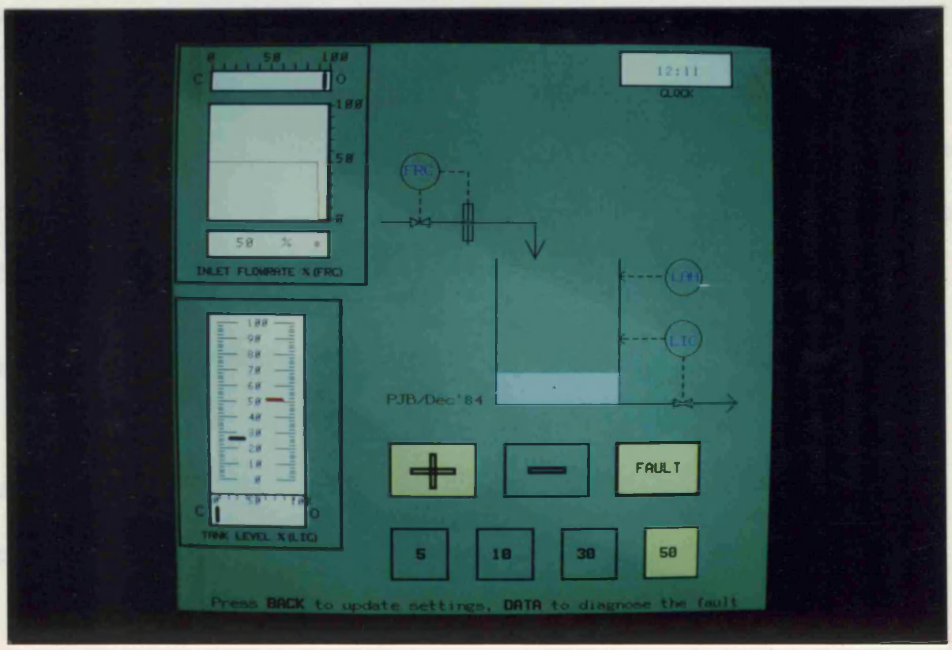


Figure 7.30 : Tank Level Control Fault Simulation



The current flowrate setpoint is displayed in the box beneath the chart. The tank level is shown on an indicator-controller in terms of a percentage of the tank's depth. The current level is shown by the left hand pointer whilst the right hand pointer shows the setpoint. The controller output signal to the valve is shown as a percentage beneath the indicator.

An animated display of the tank level control system is shown on the right hand side of the screen together with a number of touch panel option boxes. These allow the trainee to change the setpoints of the controllers and introduce process faults and disturbances into the simulation. Figure 7.29 shows the start-up of the system. By changing setpoints and observing the response on the mimic display, the trainee can investigate the response of the system at various controller settings. He can modify the settings at any time by suspending the simulation and returning to the display shown in Figure 7.28. Once he has re-specified the settings he can then return to the simulation at exactly the same point at which it was suspended but with the controller settings changed. In this way, he can go through the process of 'tuning' the process controllers using traditional 'rules of thumb' to obtain the optimum settings.

Figure 7.30 gives an example of introducing a process fault or disturbance into the simulation. This shows the effect of the inlet flow control valve failing shut. The trainee can then go through the process of diagnosing its cause as described in section 7.2.1.4.

If at any time the level in the tank is taken above 90% of the tank's depth then a 'HIGH LEVEL' alarm is displayed on the screen. In the event of the tank over-flowing, the simulation is tripped and the trainee is given feedback on his actions. This situation normally occurs if the controller settings are incorrect, unless the level has been taken high deliberately, and so at this point the trainee is able to obtain information on the optimum controller settings.

7.4 Continuous Stirred Tank Reactor Control

7.4.1 Introduction

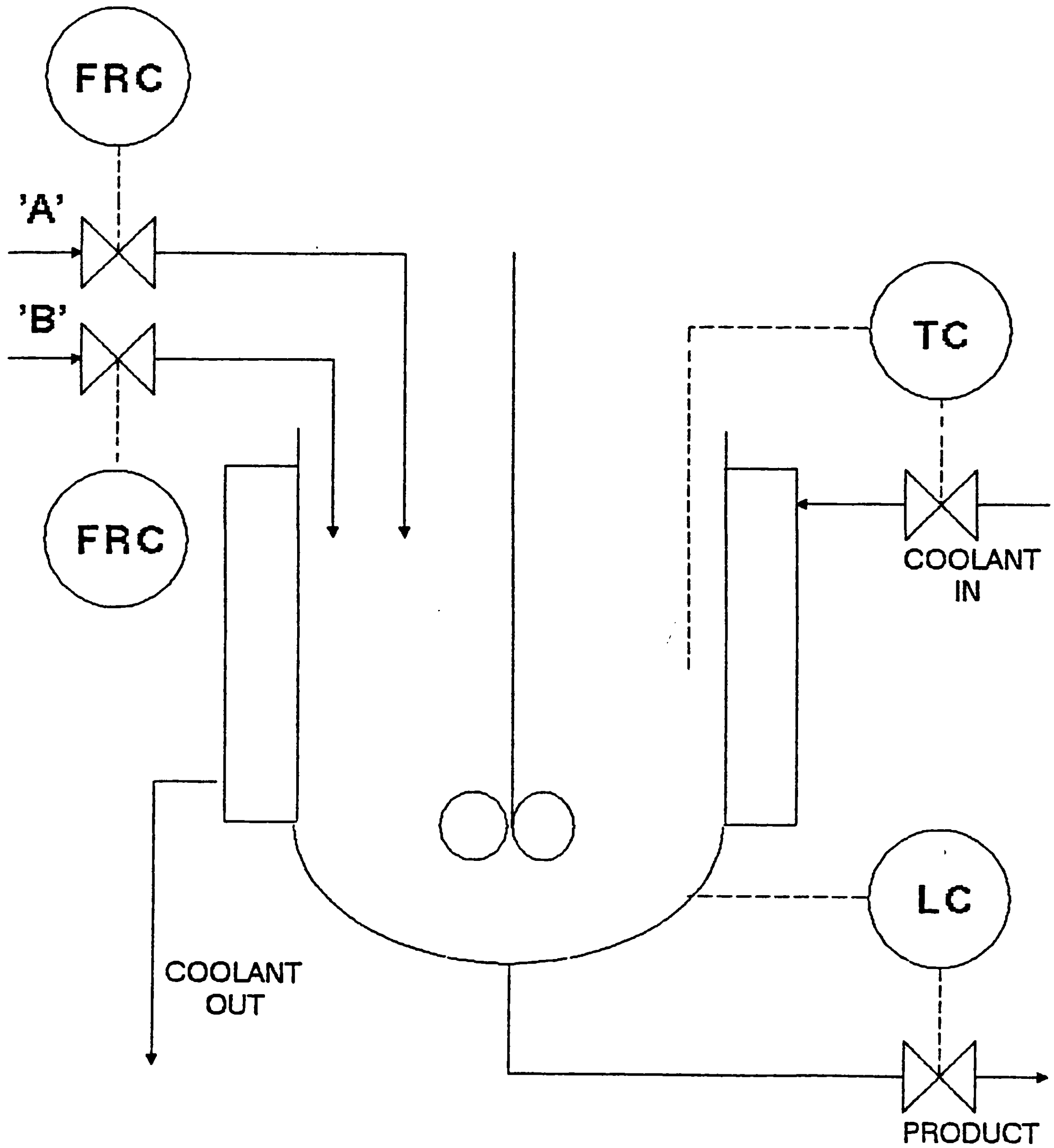
This program simulates the operation and control of a continuous stirred tank reactor, in which an exothermic reaction is taking place as follows(Y1) :-

$$A + B \rightleftharpoons C \qquad \text{.......(7.18)}$$

The control system shown in Figure 7.31 consists of a stirred tank which is continuously fed with the two aqueous reactants 'A' and 'B'. The feedrate of each reactant is controlled by a proportional + integral action controller. The reaction products are removed from the reactor through a flow control valve which is adjusted by a third P + I controller, LC. This controls the level of liquid in the reactor vessel.

The temperature of the reactor is also controlled by a fourth P + I level controller, TC which regulates the flow of coolant to the reactor cooling jacket.

Figure 7.31 : Continuous Stirred Tank Reactor Control System



The objectives of the simulation are :-

(a) To demonstrate the operation of a continuous stirred tank reactor control system.

(b) To demonstrate the use of some typical modern process control computer displays.

(c) To demonstrate the effect of some common process faults and disturbances on a typical reactor control system.

(d) To give practice in fault diagnosis.

The structure of the program is similar to that given in Figure 6.1. The 'USE' language code for the continuous stirred tank reactor control program is given in lessons 'reacint' and 'reacsim' in Appendix 3.6. A brief description of the program as seen by the trainee is given in section 7.4.3. First of all a description of the equations which model the system is given in the next section 7.4.2.

7.4.2 Mathematical Model

The continuous stirred tank reactor is assumed to be ideally mixed and therefore the temperature and composition of the product stream leaving the reactor is taken to be the same as that found at any point within the reactor. It is also assumed that the cooling jacket is ideally mixed, so that the temperature throughout the cooling jacket is the same as the coolant exit temperature and that there is negligible heat loss from the vessel.

Consider the system shown in Figure 7.31 an overall material balance over the reactor can be written as follows :-

$$\frac{dHr}{dt} = \frac{Fa + Fb - Fc}{\rho * Ar} \quad ....(7.19)$$

where Fa = mass flowrate of reactant 'A'

Fb = mass flowrate of reactant 'B'

Fc = mass flowrate of product

ρ = average bulk density of reaction mass

Ar = cross sectional area of reactor

Hr = liquid level in reactor

Similarly, material balances can be written for each of the reactants :-

$$Hr * Ar * \rho * \frac{dCar}{dt} = Fa * Ca - Fc * Car - Ra \quad ....(7.20)$$

$$Hr * Ar * \rho * \frac{dCbr}{dt} = Fb * Cb - Fc * Cbr - Rb \quad ....(7.21)$$

$$Hr * Ar * \rho * \frac{dCcr}{dt} = - Fc * Ccr + Rc \quad ....(7.22)$$

where Ca = mass fraction of reactant 'A' in feed

Cb = mass fraction of reactant 'B' in feed

Car = mass fraction of reactant 'A' in reactor

Cbr = mass fraction of reactant 'B' in reactor

Ccr = mass fraction of reactant 'C' in reactor

Ra = mass rate of consumption of reactant 'A'

Rb = mass rate of consumption of reactant 'B'

Rc = mass rate of generation of product 'C'

The feed flowrate of reactant 'A' is dependent on the supply pressure, Pa as follows :-

$$Fa = FaCv * \sqrt{Pa} \qquad ....(7.23)$$

where FaCv = Reactant 'A' flow control valve discharge coefficient

Similarly, the feed flowrate of reactant 'B' can be calculated as follows :-

$$Fb = FbCv * \sqrt{Pb} \qquad ....(7.24)$$

where FbCv = Reactant 'B' flow control valve discharge coefficient

Pb = Reactant 'B' supply pressure

The flowrate of product out of the reactor can be related to the level of liquid in the vessel :-

$$Fc = lCv * \sqrt{Hr} \qquad ....(7.25)$$

where lCv = reactor discharge flow control valve coefficient

Now considering the rate of reaction for the reaction :-

$$A + B \underset{k2}{\overset{k1}{\rightleftharpoons}} C \qquad ....(7.18)$$

where k1 = forward reaction rate constant

k2 = reverse reaction rate constant

For an elementary reaction scheme, the reaction rate can be expressed in terms of moles per unit volume as follows :-

$$\frac{d[A]}{dt} = k2 * [C] - k1 * [A] * [B] \qquad ....(7.26)$$

where [A] = molar concentration of reactant 'A' in reactor

[B] = molar concentration of reactant 'B' in reactor

[C] = molar concentration of product 'C' in reactor

From the stochiometry of the reaction,

$$\frac{d[A]}{dt} = \frac{d[B]}{dt} = \frac{-d[C]}{dt} \qquad ....(7.27)$$

For a non-isothermal reaction the rate constants are dependent on the reaction temperature by Arrhenius expressions as follows :-

$$k1 = A1 * \exp(-B1/Tr) \qquad ....(7.28)$$

$$k2 = A2 * \exp(-B2/Tr) \qquad ....(7.29)$$

where Aj, Bj are constants

Therefore the molar rate of consumption per unit volume of reactant 'A' can be calculated from equations 7.26, 7.28 and 7.29. The mass reaction rates can then be calculated as follows using equation 7.27 :-

$$Ra = MWa * Hr * Ar * \frac{d[A]}{dt} \qquad ....(7.30)$$

$$Rb = MWb * Hr * Ar * \frac{d[A]}{dt} \qquad ....(7.31)$$

$$Rc = MWc * Hr * Ar * \frac{-d[A]}{dt} \qquad ....(7.32)$$

where MWj = molecular weight of component j

Now consider heat balances over reactor and its heating jacket to determine the reaction temperature, Tr. First of all consider a heat balance over the reactor :-

$$\frac{dTr}{dt} = \frac{Fa * Cp * Ta + Fb * Cp * Tb - Fc * Cp * Tr + Qr - q}{\rho * Ar * Hr * Cp} \qquad \text{.......(7.33)}$$

where Cp = average specific heat capacity of the reaction mixture

Ta = temperature of feed stream of component 'A'

Qr = total heat of reaction = Ra $*\Delta$H ....(7.34)

ΔH = heat of reaction per unit mass of component 'A'

q = rate of heat transfer from reactor to cooling jacket = Ur * Aht * (Tr - Tj) ....(7.35)

Ur = overall heat transfer coefficient

Aht = heat transfer area

Tj = coolant temperature in the cooling jacket

Similarly, a heat balance can also be written for the cooling jacket as follows :-

$$\frac{dTj}{dt} = \frac{Fj * Cpj * (Ti - Tj) + q}{Mj * Cpj} \qquad \text{.......(7.36)}$$

where Fj = mass flowrate of coolant fed to cooling jacket

Cpj = average specific heat capacity of coolant

Ti = temperature of coolant fed to cooling jacket

Mj = mass of coolant in cooling jacket

The equations can then be solved using the algorithm shown in Figure 6.2 and described in section 6.4.2. Equations 7.23, 7.24, 7.25, 7.26, 7.28, 7.29, 7.30, 7.31, 7.32, 7.34 and 7.35 are the algebraic equations and equations 7.19, 7.20, 7.21, 7.22, 7.33 and 7.36 contain the time dependent derivatives. The integration is carried out using the 'intin' and 'intde' routines described in Appendix 2.

The action of the four controllers for the reactant feed flowrates and the reactor level and temperture are modelled using the 'PIcontr' routine. The discharge coefficients of the four associated control valves are modelled using the 'valve' routine. These routines are also described in Appendix 2.

The program includes eight process faults and disturbances and these are listed in Table 7.4. The faults are simulated in a similar way to those described for the steam-heated heat exchanger in section 7.2.1.3. The 'USE' language code for the simulation calculations are given in section 'simcalcs' and for the fault simulation in section 'fault' of the lesson 'reacsim' given in Appendix 3.6.

Table 7.4 Continuous Stirred Tank Reactor Control Process Faults and Disturbances.

Process Faults And Disturbances
1. Fouling of cooling jacket
2. Decrease in reactant 'A' inlet flow supply pressure
3. Decrease in reactant 'B' inlet flow supply pressure
4. Reactor outlet flow control valve failed open
5. Reactor outlet flow control valve jammed
6. Reactant feed temperature change
7. Reactant feed concentration change
8. Reactor cooling jacket flow control valve failed open

7.4.3 The Program as Seen by the Trainee

A sample of the continuous stirred tank reactor control program screen displays as seen by the trainee are given in Figures 7.32 to 7.34. The animated mimic control panel displays were developed to be representative of the style of computer displays used in modern process control systems(L11).

Figure 7.32 shows the main process diagram display. It features a diagram of the plant equipment with the values of the measured and controlled variables displayed at the appropriate points. At the bottom of the display there are a number of touch panel boxes which allow the trainee to change the setpoint of each controller and to introduce random faults and disturbances.

Figure 7.32 : Continuous Stirred Tank Reactor Control
Overall Process Display

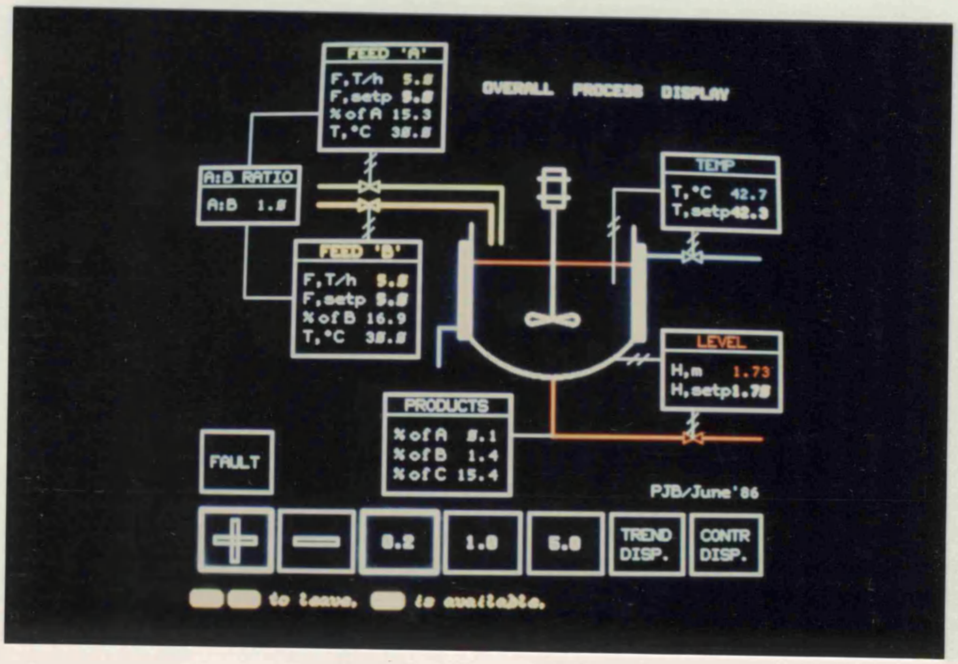


Figure 7.33 : Continuous Stirred Tank Reactor Control
Controller Display

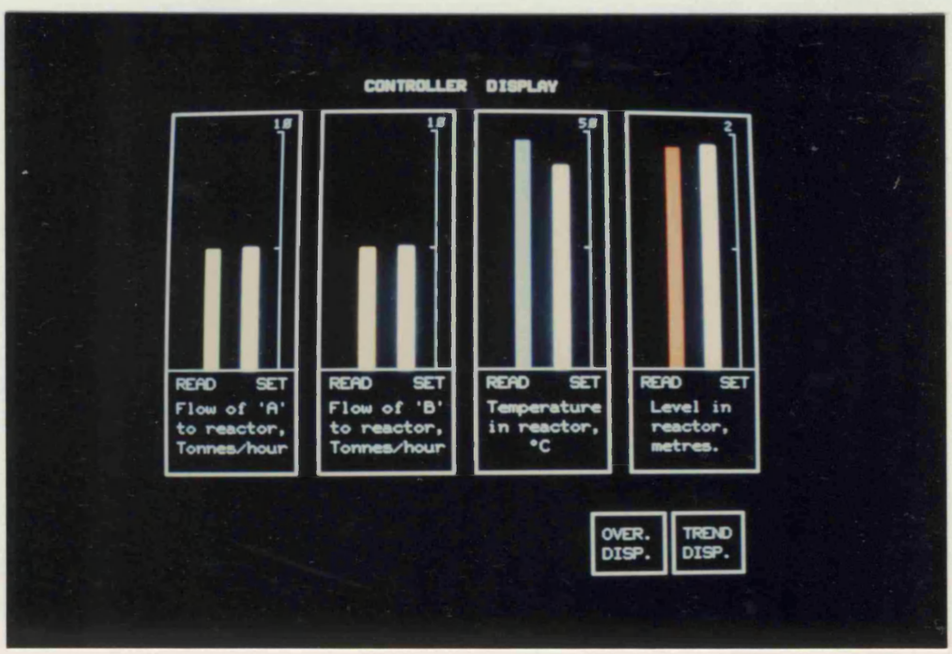
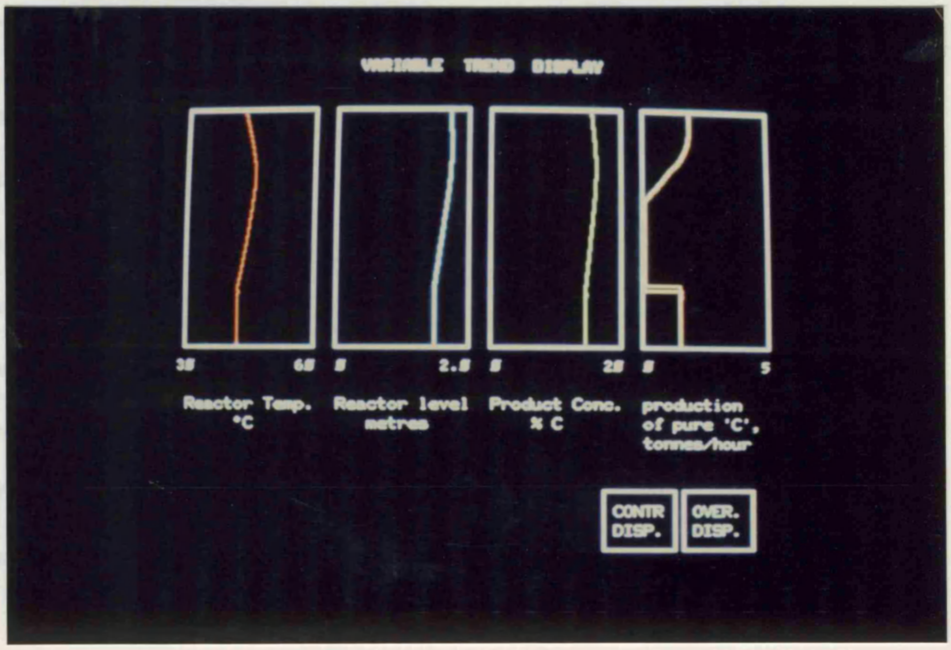


Figure 7.34 : Continuous Stirred Tank Reactor Control
Variable Trend Display



The trainee can obtain help on operating the simulation at any time by pressing the 'help' key and he can also switch to one of two other mimic control panel displays.

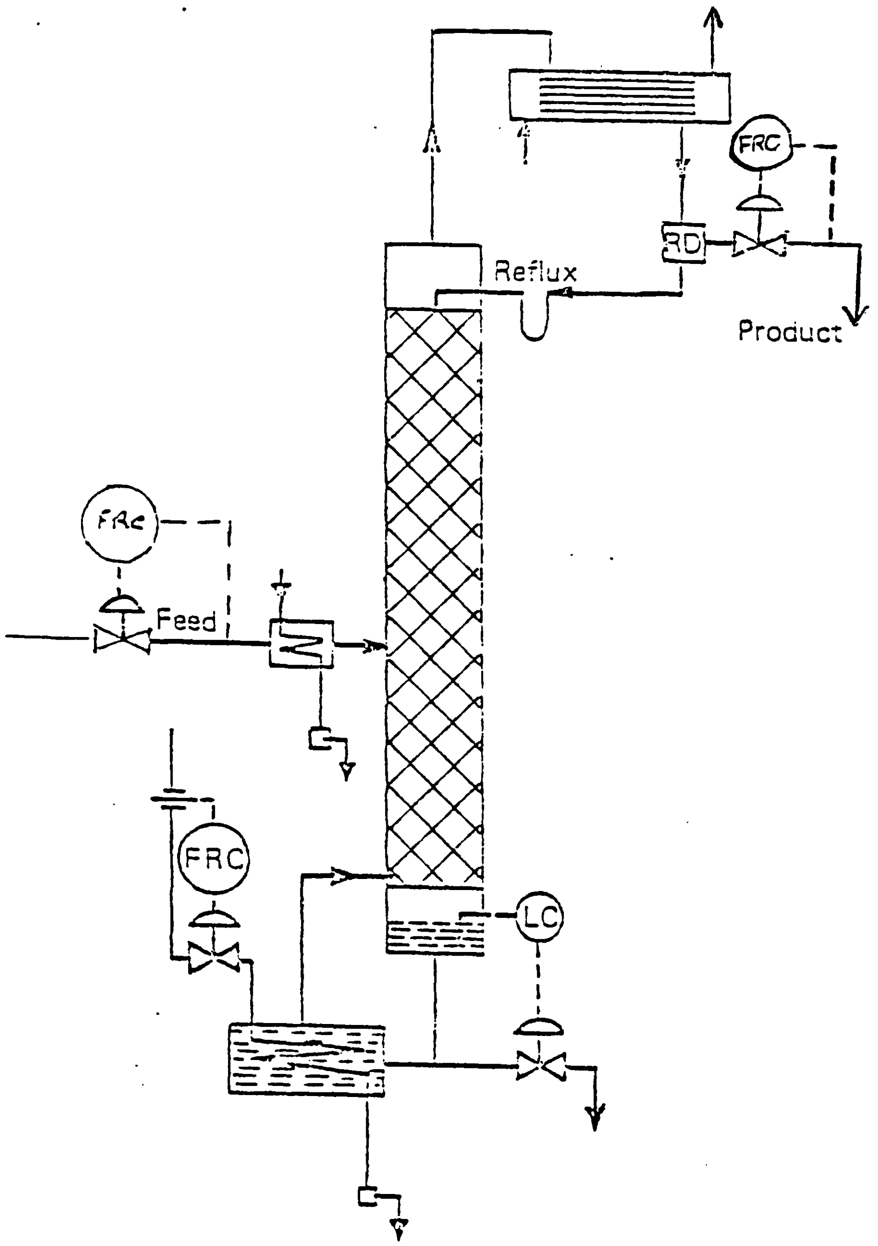
Figure 7.33 shows the controller display which features bar charts of the controller setpoints compared to the current measured values of the controlled variables. The third mimic control panel display is shown in Figure 7.34. This shows the variable trend display which presents the variation of four of the main process variables with time. Figures 7.32 to 7.34 show the effect of a step change in the value of the level setpoint.

7.5 Continuous Binary Distillation Control

7.5.1 Introduction

This program simulates the operation and control of a continuous binary distillation column(Y2). The distillation column control system shown in Figure 7.35 consists of a liquid mixture of 80% acetone and 20% ethanol at its bubble point being fed to a plate column consisting of 18 theoretical equilibrium stages. The liquid feedrate to the column is controlled by a proportional + integral action controller. The vapour from the column head is condensed in a total condenser. The liquid distillate flowrate is adjusted by a second P + I controller and this in turn varies the reflux returned to the column.

Figure 7.35 : Continuous Binary Distillation Control System



The level of liquid in the column bottom is controlled by a P + I level controller, LC which opens and closes the bottom product flow control valve accordingly. The bottoms liquid is boiled by heat exchange with saturated steam in an external reboiler. The flow of steam to the reboiler is controlled by a fourth P + I controller.

This control scheme does not reflect a typical distillation column configuration since it does not include quality control on the top and bottom products. The scheme was chosen by plant management to enable the trainee to easily investigate the following training objectives. The objectives of the simulation are :-

(a) To show the effect of boil-up rate on column temperatures and product composition.

(b) To show the effect of feed rate on column temperatures and product composition.

(c) To show the effect of reflux ratio on column temperatures and product composition.

(d) To demonstrate the operation of a continuous distillation control system.

The structure of the program is similar to that given in Figure 6.1 with the fault options being unavailable. The 'USE' language code for the distillation control program is given in lesson 'distsim' in Appendix 3.7. A brief description of the program as seen by the trainee is given in section 7.5.3. First of all a description of the equations which model the system is given in the next section 7.5.2.

7.5.2 Mathematical Model

The following assumptions will be made in deriving the mathematical model of the operation of the distillation column control system which is based on similar models presented by Deshpande(D9) and Wei(W5) :-

(a) Vapour hold-up is negligible.

(b) Liquid and vapour are well mixed on each tray.

(c) Tray effluent streams are in thermodynamic equilibrium.

(d) Column pressure assumed constant.

(e) Thermal capacity of the column and trays is negligible.

(f) Tray thermal dynamics are assumed to be rapid so that the energy equation reduces to an algebraic equation.

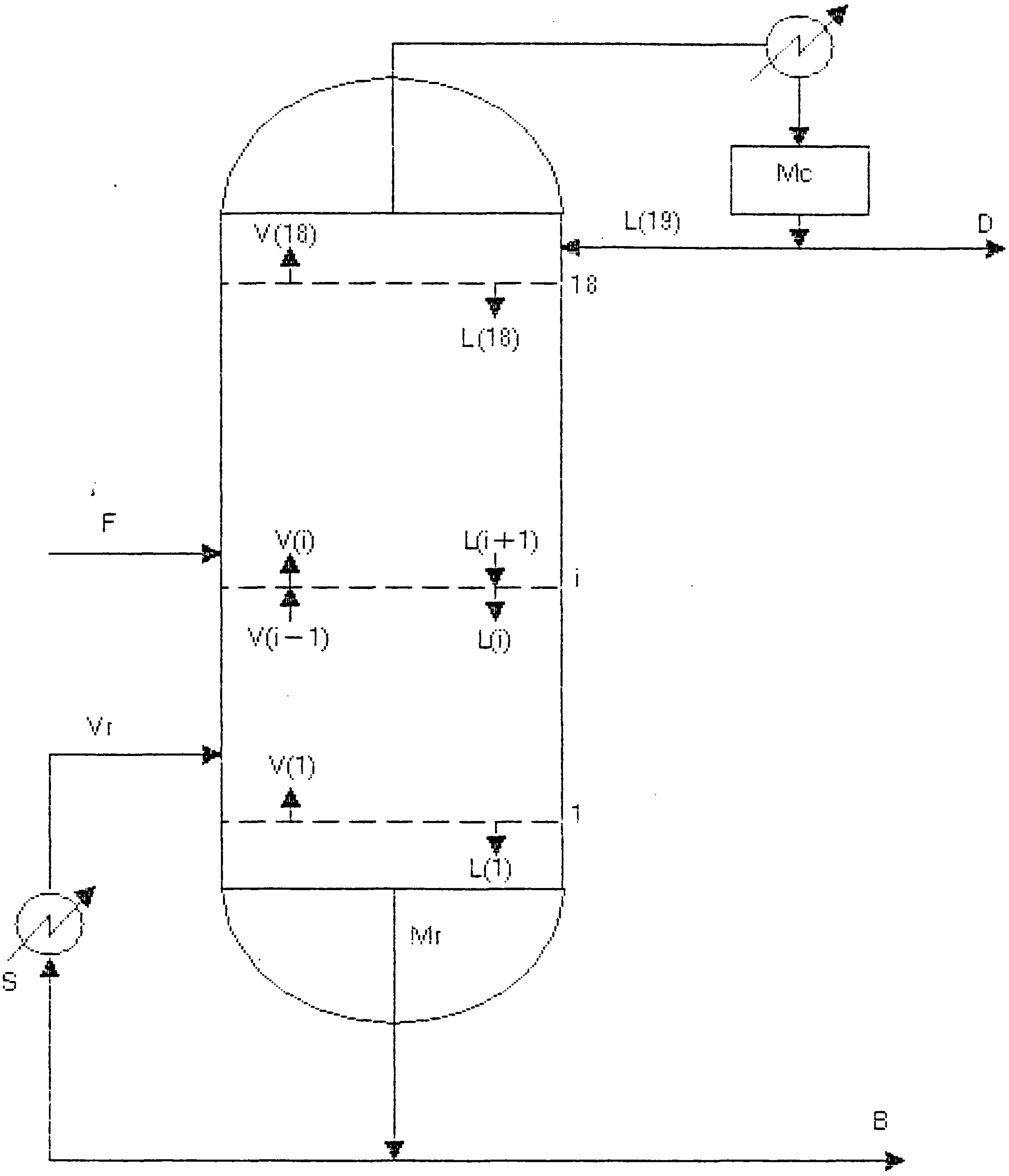
(g) Tray efficiency is constant.

(h) Thermal dynamics of reboiler and condenser are assumed to be negligible.

(i) Reboiler hold-up is negligible compared to column bottom.

Consider the schematic diagram of the distillation column in Figure 7.36. This is based on the assumptions and simplifications listed above and shows the tray numbering system.

Figure 7.36 : Continuous Binary Distillation Model



Considering the reboiler, ordinary differential equations can be written to describe the variation of the total and component bottoms liquid hold-up :-

$$\frac{dMr}{dt} = L(1) - B - Vr \qquad ....(7.37)$$

$$\frac{dXMr}{dt} = Xa(1) * L(1) - Xar * B - Yar * Vr \qquad ....(7.38)$$

where Mr = total liquid molar hold-up in column bottom

XMr = acetone liquid molar hold-up in column bottom

L(1) = total liquid molar flowrate from 1st tray

Xa(1) = acetone liquid mole fraction from 1st tray

B = bottoms liquid molar flowrate

Xar = bottoms acetone liquid mole fraction

Vr = total vapour molar flowrate from reboiler

Yar = acetone vapour mole fraction from reboiler

The bottoms liquid molar flowrate is dependent on the amount of hold-up in the column bottom as follows :-

$$B = lCv * \sqrt{Mr} \qquad ....(7.39)$$

where lCv = bottoms liquid flow control valve coefficient

The new bottoms acetone liquid mole fraction can then be calculated from :-

$$Xar = XMr / Mr \qquad ....(7.40)$$

Correlations were derived from data using the routine 'curve' described in the 'simpac' manual in Appendix 2 for the equilibrium relationships between acetone mole fraction in the liquid, Xa and acetone mole fraction in the vapour, Ya and equilibrium temperature, T :-

$$Xa = a2 * Ya^2 + a1 * Ya + a0 \qquad ....(7.41)$$

$$T = b2 * Xa^2 + b1 * Xa + b0 \qquad ....(7.42)$$

where a2, a1, a0, b2, b1, b0 are constants

Using these relationships, the temperature in the reboiler, Tr and the equilibrium mole fraction of the vapour leaving the reboiler, Yar can be determined.

The heat load on the reboiler, Qr is dependent on the steam molar flowrate, S :-

$$Qr = S * Hvap \qquad ....(7.43)$$

where Hvap = latent heat of vaporisation of saturated steam @ 2 atm, 120 C

The steam molar flowrate is obtained from :-

$$S = sCv * \sqrt{(Ps1 - Ps2)} \qquad ....(7.44)$$

where sCv = steam flow control valve coefficient

Ps1 = steam supply pressure

Ps2 = steam pressure in reboiler

The new total vapour molar flowrate, Vr returned to the column from the reboiler can be determined from an enthalpy balance over the column bottom as follows :-

$$Vr = \frac{L(1) * h(1) - B * hb + Qr}{Hr} \qquad ....(7.45)$$

where h(1) = specific enthalpy of liquid from 1st tray

hb = specific enthalpy of bottoms liquid

Hr = specific enthalpy of vpaour from reboiler

Considering the 1st tray shown in Figure 7.36, ordinary differential equations can be written to describe the variation of the total and component tray liquid hold-up :-

$$\frac{dM(1)}{dt} = L(2) + Vr - L(1) - V(1) \qquad ....(7.46)$$

$$\frac{dXM(1)}{dt} = Xa(2) * L(2) + Yar * Vr - Xa(1) * L(1) - Ya(1) * V(1) \qquad ....(7.47)$$

where M(1) = total liquid molar hold-up on 1st tray

XM(1) = acetone liquid molar hold-up on 1st tray

L(2) = total liquid molar flowrate from 2nd tray

Xa(2) = acetone liquid mole fraction from 2nd tray

V(1) = total vapour molar flowrate from 1st tray

Ya(1) = acetone vapour mole fraction from 1st tray

The new acetone liquid mole fraction from the 1st tray can then be calculated from :-

$$Xa(1) = XM(1) / M(1) \qquad ....(7.48)$$

The new liquid molar flowrate from the 1st tray can then be calculated using a modified Francis Weir equation :-

$$L(1) = C1 * M(1)^{1.5} + C2 \qquad ....(7.49)$$

where C1, C2 are constants

Equations 7.41 and 7.42 can then be used to determine the tray equilibrium temperature, T(1) and the acetone mole fraction of vapour from the tray, Ya(1).

The new vapour molar flowrate from the 1st tray can then be calculated from a tray enthalpy balance :-

$$V(1) = \frac{Vr * Hr + L(2) * h(2) - L(1) * h(1)}{H(1)} \qquad ....(7.50)$$

where h(2) = specific enthalpy of liquid from 2nd tray

H(1) = specific enthalpy of vapour from 1st tray

The remaining theoretical equilibrium stages except the feed tray can be modelled using a series of generalised equations. Considering the ith tray shown in Figure 7.36, ordinary differential equations can be written to describe the variation of the total and component tray liquid hold-up :-

$$\frac{dM(i)}{dt} = L(i+1) + V(i-1) - L(i) - V(i) \qquad ....(7.51)$$

$$\frac{dXM(i)}{dt} = Xa(i+1) * L(i+1) + Y(i-1) * V(i-1) - Xa(i) * L(i) - Ya(i) * V(i) \qquad ....(7.52)$$

where $M(i)$ = total liquid molar hold-up on ith tray

$XM(i)$ = acetone liquid molar hold-up on ith tray

$L(i)$ = total liquid molar flowrate from ith tray

$Xa(i)$ = acetone liquid mole fraction from ith tray

$V(i)$ = total vapour molar flowrate from ith tray

$Ya(i)$ = acetone vapour mole fraction from ith tray

The new acetone liquid mole fraction from the ith tray can then be calculated from :-

$$Xa(i) = XM(i) / M(i) \qquad \qquad ....(7.53)$$

The new liquid molar flowrate from the ith tray can then be calculated using a modified Francis Weir equation as before :-

$$L(i) = C1 * M(i)^{1.5} + C2 \qquad \qquad ....(7.54)$$

where C1, C2 are constants

Equations 7.41 and 7.42 can then be used to determine the tray equilibrium temperature, T(i) and the acetone mole fraction of vapour from the tray, Ya(i).

The new vapour molar flowrate from the ith tray can then be calculated from a tray enthalpy balance :-

$$V(i) = \frac{V(i-1) * H(i-1) + L(i+1) * h(i+1) - L(i) * h(i)}{H(i)} \qquad ....(7.55)$$

where $h(i)$ = specific enthalpy of liquid from ith tray

$H(i)$ = specific enthalpy of vapour from ith tray

Considering the feed tray, ordinary differential equations can be written as before to describe the variation of the total and component tray liquid hold-up :-

$$\frac{dM(i)}{dt} = L(i+1) + V(i-1) + F - L(i) - V(i) \qquad \text{.......(7.56)}$$

$$\frac{dXM(i)}{dt} = Xa(i+1) * L(i+1) + Xaf * F + Y(i-1) * V(i-1)$$
$$- Xa(i) * L(i) - Ya(i) * V(i) \qquad \text{.......(7.57)}$$

where Xaf = acetone liquid mole fraction in the feed

F = total feed molar flowrate

The total molar feed flowrate, F is determined from :-

$$F = fCv * \sqrt{Pf1 - Pf2} \qquad \text{.......(7.58)}$$

where fCv = feed flow control valve coefficient

Pf1 = feed supply pressure

Pf2 = column pressure

The new acetone liquid mole fraction and molar flowrate from the feed tray can be calculated using equations 7.53 and 7.54 as before. Equations 7.41 and 7.42 can then be used to determine the tray equilibrium temperature, T(i) and the acetone mole fraction of vapour from the tray, Ya(i).

The new vapour molar flowrate from the feed tray can then be calculated from a tray enthalpy balance :-

$$V(i) = (V(i-1) * H(i-1) + L(i+1) * h(i+1)$$
$$+ F * hf - L(i) * h(i)) / H(i) \qquad \text{.......(7.59)}$$

where hf = specific enthalpy of feed liquid

Finally, considering the total condenser shown in Figure 7.36, ordinary differential equations can be written to describe the total and component molar hold-up :-

$$\frac{dMc}{dt} = V(18) - D - L(19) \qquad ....(7.60)$$

$$\frac{dXMc}{dt} = Ya(18) * V(18) - Xad * D - Xa(19) * L(19) \qquad ....(7.61)$$

where Mc = total liquid molar hold-up in total condenser

XMc = acetone liquid molar hold-up in total condenser

D = total distillate liquid molar flowrate

Xad = acetone distillate liquid mole fraction

V(18) = total vapour molar flowrate from 18th tray

Ya(18) = acetone vapour mole fraction from 18th tray

L(19) = liquid molar flowrate returned to the column

Xa(19) = acetone liquid mole fraction returned to the column

The new acetone liquid mole fraction from the total condenser can then be calculated from :-

$$Xad = Xa(19) = XMc / Mc \qquad ....(7.62)$$

The distillate molar liquid flowrate, D is dependent on the condenser hold-up, Mc as follows :-

$$D = dCv * \sqrt{Mc} \qquad ....(7.63)$$

where dCv = distillate flow control valve coefficient

Similarly, the liquid flowrate returned to the column is also dependent on the condenser hold-up :-

$$L(19) = cCv * \sqrt{Mc} \qquad \qquad ....(7.64)$$

where cCv = condenser discharge coefficient

These equations can then be solved using the algorithm shown in Figure 6.2 and described in section 6.4.2. The equations are solved in six sections starting with the reboiler. For the reboiler, equations 7.39, 7.40, 7.41, 7.42, 7.43, 7.44 and 7.45 are the algebraic equations and equations 7.37 and 7.38 are the time dependent derivatives. For the bottom tray, equations 7.41, 7.42, 7.48, 7.49 and 7.50 are the algebraic equations and equations 7.47 and 7.48 are the time dependent derivatives. For the the rest of the trays in the column except the feed tray, equations 7.41, 7.42, 7.53, 7.54 and 7.55 are the algebraic equations and equations 7.51 and 7.52 contain the time dependent derivatives. For the feed tray, equations 7.41, 7.42, 7.53, 7.54, 7.58 and 7.59 are the algebraic equations and equations 7.56 and 7.57 are the time dependent derivatives. Finally for the total condenser, equations 7.62, 7.63 and 7.64 are the algebraic equations and equations 7.60 and 7.61 are the time dependent derivatives. The integration is carried out using the 'intin' and 'intde' routines described in Appendix 2.

Checks are included in the calculations to ensure that values of acetone mole fraction do not exceed the physical values of 0 or 1.0 and similarly values of hold-up are not calculated to be negative. It is important that the program exhibits a high degree of robustness. Routines are included in the program to calculate the liquid and vapour enthalpies of acetone-ethanol mixtures. These are determined as follows assuming that there is no heat of mixing :-

$$H(i) = Ya(i) * Ha(i) + (1 - Ya(i)) * He(i) \qquad ....(7.65)$$

$$h(i) = Xa(i) * ha(i) + (1 - Xa(i)) * he(i) \qquad ....(7.66)$$

where Ha(i) = vapour specific enthalpy of acetone

He(i) = vapour specific enthalpy of ethanol

ha(i) = liquid specific enthalpy of acetone

he(i) = liquid specific enthalpy of ethanol

An initial estimate of the tray temperature, liquid flowrate and acetone mole fraction profiles within the column is required before the simulation can be run. A process design simulation package, 'Chemcad' was run to obtain the steady-state column profiles for a given feedrate and top and bottom acetone mole fraction specification. 'Chemcad' is described by Baker-Counsell(B10). This data was then entered into the simulation and 'tuned' to obtain the initial set of profiles required.

The action of the four controllers for the liquid feedrate to the column, the liquid distillate flowrate, the liquid bottoms flowrate and the steam flowrate to the reboiler are modelled using the 'PIcontr' routine. The discharge coefficients of the four associated control valves are modelled using the 'valve' routine. These routines are also described in Appendix 2. The 'USE' language code for the simulation calculations are given in section 'simcalcs' of the lesson 'distsim' given in Appendix 3.7.

7.5.3 The Program as Seen by the Trainee

A sample of the continuous binary distillation control program screen displays as seen by the trainee are given in Figures 7.37 to 7.41. The animated mimic control panel displays were developed to be representative of the style of computer displays used in modern process control systems(L11).

Figure 7.37 shows the main process diagram display. It features a diagram of the plant equipment with the values of the measured and controlled variables displayed at the appropriate points. At the bottom of the display there is a number of touch panel boxes which allow the trainee to change the mode of operation, either manual or automatic of each controller. He can also change the controller setpoint if operating in automatic mode and the valve position if operating in manual mode. The trainee can obtain help on operating the simulation at any time by pressing the 'help' key and he can also switch to one of two other mimic control panel displays.

Figure 7.37 : Continuous Binary Distillation Control
Overall Process Display

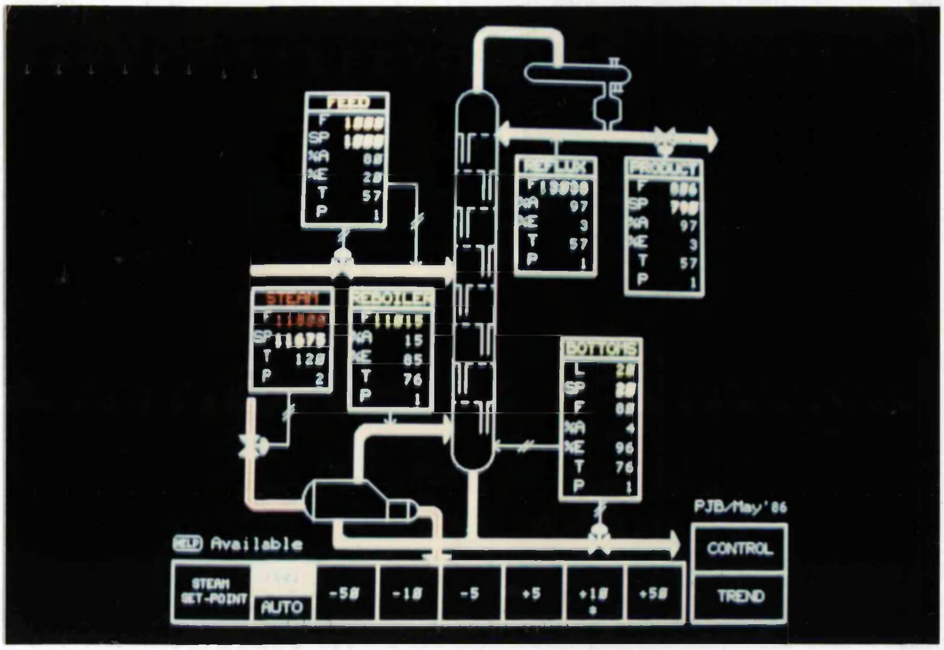


Figure 7.38 : Continuous Binary Distillation Control
Controller Display

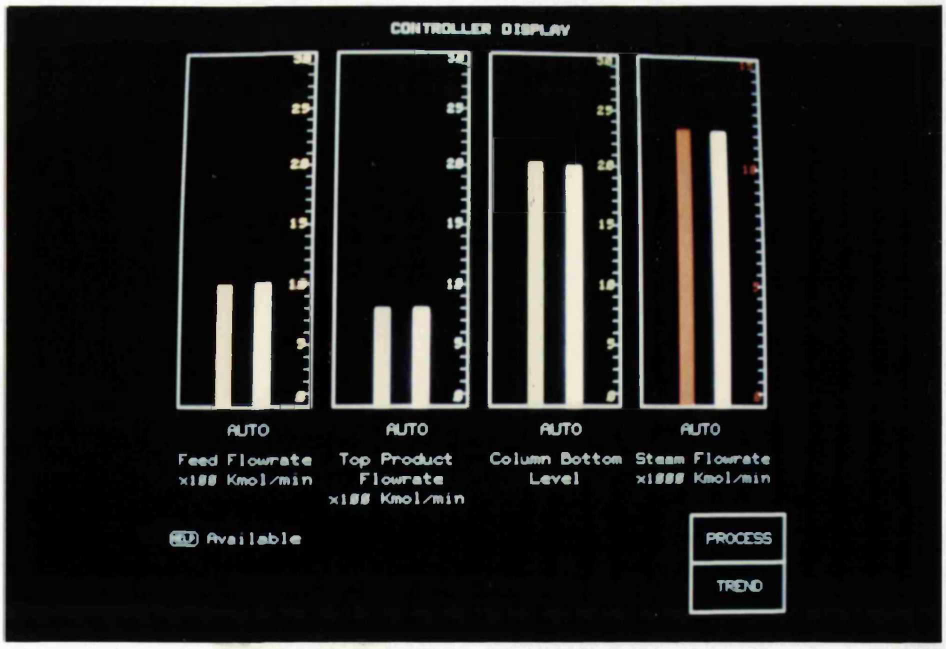


Figure 7.39 : Continuous Binary Distillation Control
Variable Trend Display

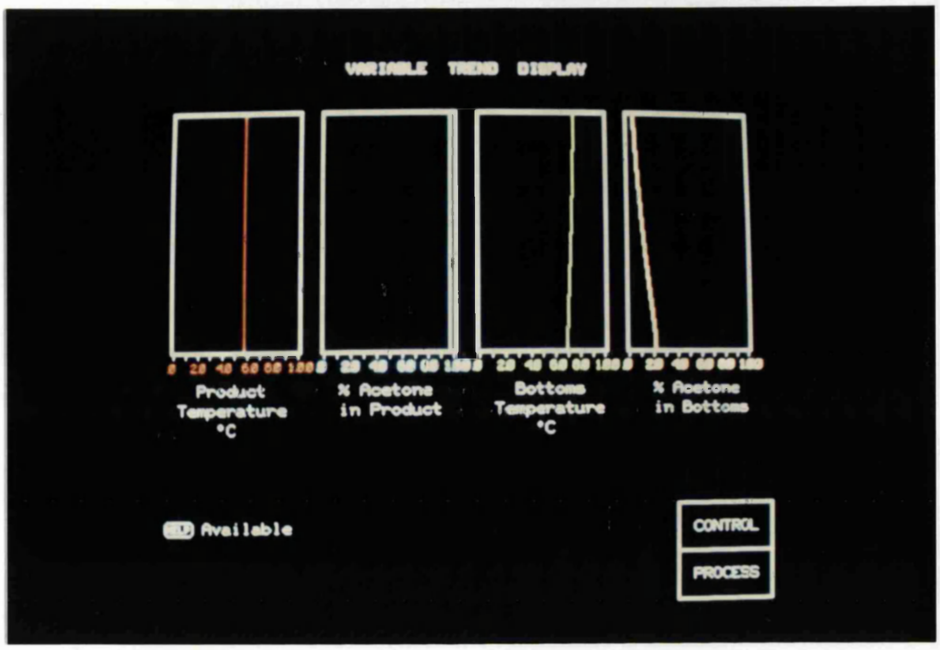


Figure 7.38 shows the controller display which features bar charts of the controller setpoints compared to the current measured values of the controlled variables. The current mode of operation of each controller is also displayed. The third mimic control panel display is shown in Figure 7.39. This shows the variable trend display which presents the variation of four of the main process variables with time.

Figures 7.37 to 7.39 show the effect of a step change in boil-up rate by changing the steam fed to the reboiler. The variable trend display in Figure 7.39 shows that the acetone concentration in the bottom product steadily decreases as the boil-up rate increases together with an associated rise in bottoms temperature.

Figure 7.40 and 7.41 show the effect of an increase in column loading by increasing the liquid feedrate. The variable trend display in Figure 7.41 shows the acetone concentration in the bottoms steadily rising with an associated drop in temperature. An increase in boil-up rate is required to 'drive' the acetone back up the column.

Figure 7.40 : Continuous Binary Distillation Control
Effect of Increase in Feedrate

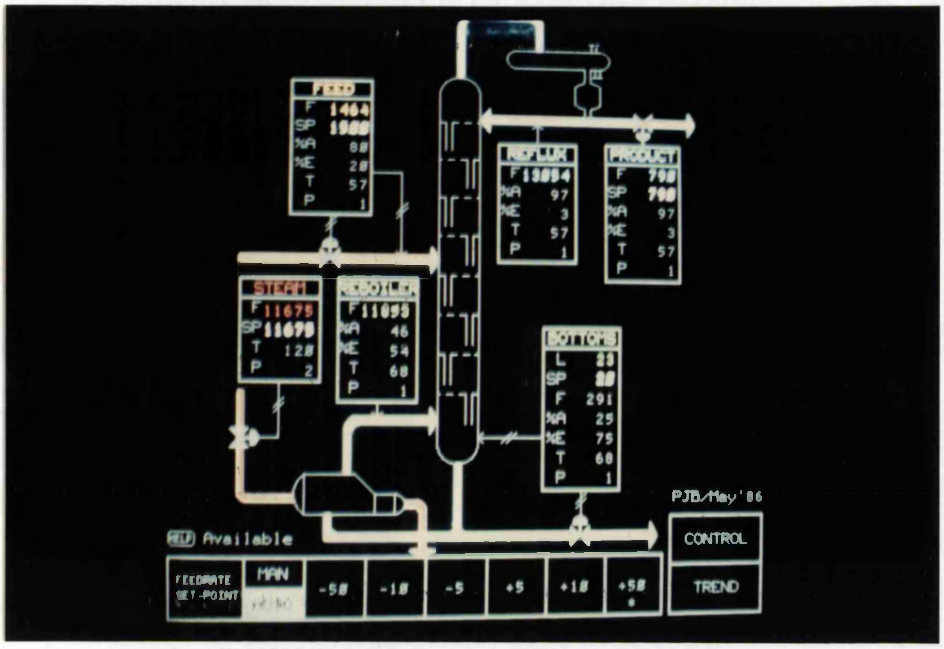
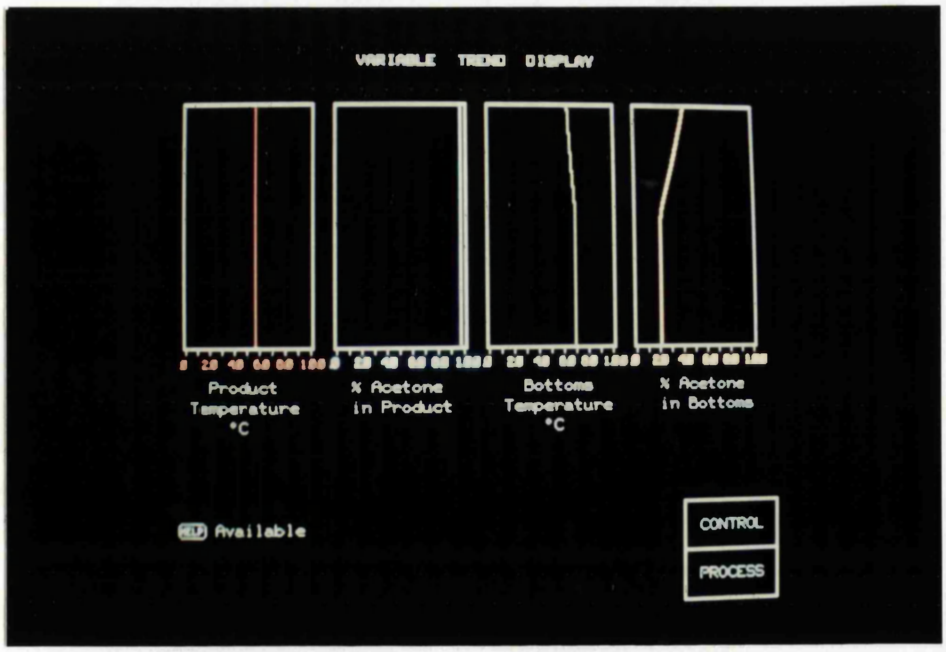


Figure 7.41 : Continuous Binary Distillation Control
Effect of Increase in Feedrate



7.6 Discussion

A number of general plant operation dynamic simulations has been presented in this chapter. It was found that these fairly simple simulations ably demonstrated the operation and control of individual unit operations. They enable the operator to gain repeated and systematic practice in control loop operation and in fault diagnosis from control panel presented information which is an important area of understanding and one which it is very difficult to train 'on-the-job'. The examples presented cover both traditional pneumatic control panel instrumentation and more modern process control computer displays. The fault diagnosis exercises include both process and instrumentation faults. The programs are particularly valuable in the initial training of control room operators because they demonstrate the principles of control without the distraction of a highly complex process.

Instrument artificers found the Tank Level Control program presented in section 7.3 particularly useful for practising their process controller tuning skills. In addition, the program allows the trainee to compare the information displayed on the control panel instruments directly with an animated flow diagram of the system.

The Manual By-Pass Heat Exchanger Control program presented in section 7.2.4 demonstrates the method of teaching an aspect of plant operation in the form of a 'game'.

It presents a challenge to the trainee and therefore stimulates him to learn by discovery.

The opinions of plant personnel were obtained from an evaluation questionnaire, the results of which are presented in Appendix 4. Table 7.5 summarises the opinions of the programs presented in this chapter. It shows that all the programs were well received. A substantial majority of those who had seen each program considered them to be either useful or very useful.

Table 7.5 General Plant Operation Dynamic Simulations Plant Personnel Opinions

	Not Useful	Useful	Very Useful
Steam-Heated Heat Exchanger Control	6%	69%	25%
Co-Current Heat Exchanger Control	6%	81%	13%
Counter-Current Heat Exchanger Control	7%	80%	13%
Manual By-Pass Heat Exchanger Control	7%	80%	13%
Tank Level Control	0	79%	21%
Continuous Stirred Tank Reactor Control	0	67%	33%

Chapter 8 Specific Plant Operation Dynamic Simulations

8.1 Introduction

This chapter presents two examples of dynamic simulations of actual plant control systems which have been used for training plant personnel. It uses the ideas presented in Chapter 6. The choice of which dynamic modelling approach to use is dependent on the quantity and quality of process data which is available. There is a great shortage of detailed dynamic process data for the plants at ICI's Severnside Works used in these examples. Therefore it is better to use an ordinary differntial equation model for each example since this will be based on the physical and chemical properties of the system. A highly accurate model is not required, just one which reproduces the plant responses to a sufficient degree of fidelity so that the training objectives can be achieved. Fairly simple ordinary differential and algebraic equation models similar to those presented in the previous Chapter 7, are used. The model parameters such as heat transfer coefficients are 'tuned' so that the performance of the models match the limited process data that are available.

A detailed description of the simulation of 'Nitric Acid Plant Ammonia Vaporiser Control' is given in the next section 8.2. It includes the simulation of some of the common process faults and disturbances associated with the system.

A brief description of the simulation of 'Ammonia Plant Make-Gas Boilers Control' is given in section 8.3.

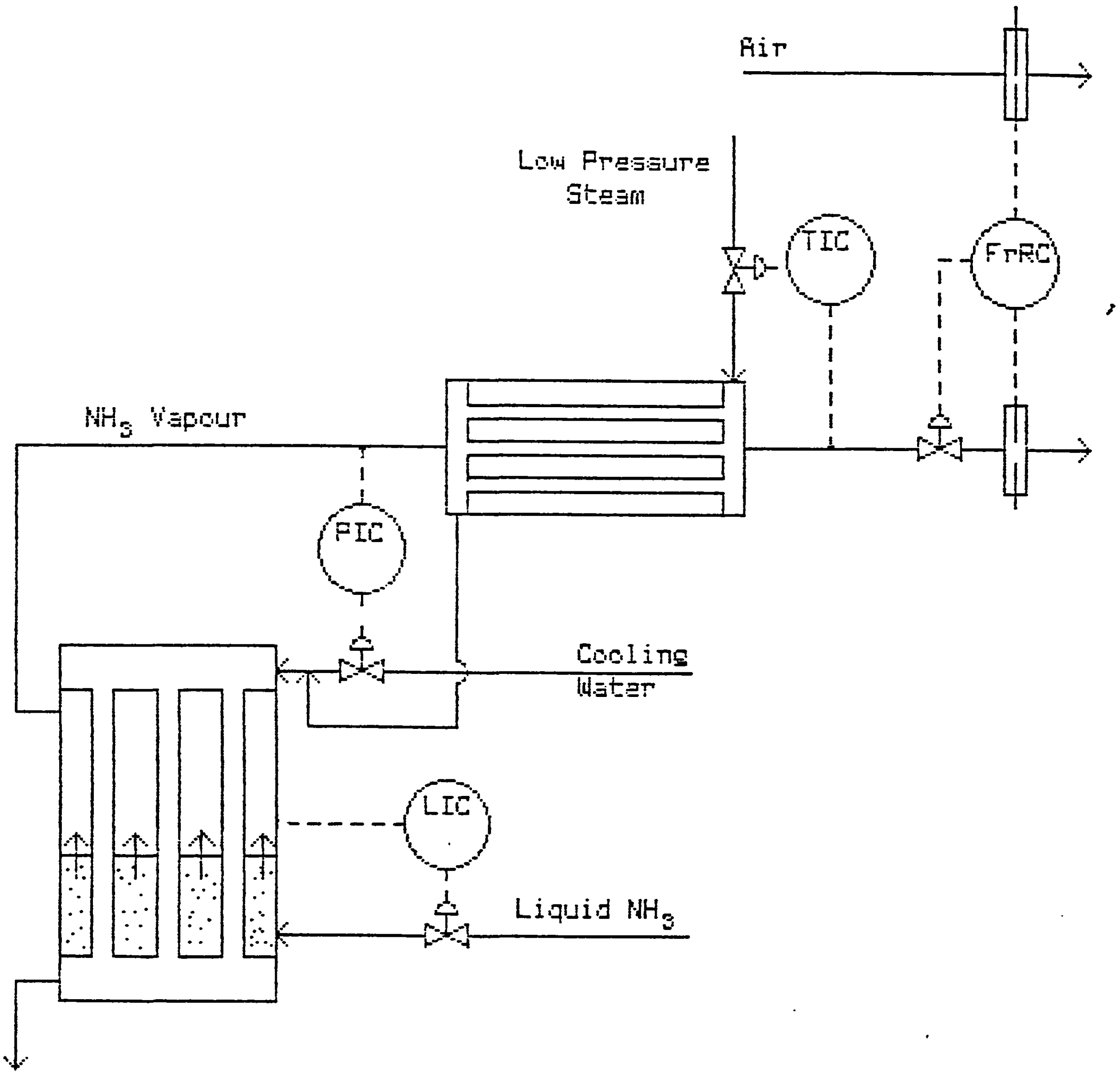
The training objectives of each example are specified in the relevant section. A comparison between the simulations and actual plant data is given and the opinions of the plant personnel of each simulation are presented. These opinions were obtained from a questionnaire, the results of which are presented in Appendix 4.

8.2 Nitric Acid Plant Ammonia Vaporiser Control

8.2.1 Introduction

This program simulates the action of the Ammonia Vaporiser control system shown in Figure 8.1(B12). It consists of a tank into which liquid ammonia is fed. The liquid level in the tank is controlled by a proportional + integral(P+I) action controller, LIC which manipulates the liquid ammonia feed flowrate. The ammonia is vaporised by heat exchange with cooling water which passes down through tubes in the vaporiser. The vaporiser pressure is controlled by a second P+I controller, PIC which adjusts the cooling water flowrate. The ammonia vapour passes to the superheater where it is heated by low pressure steam. The ammonia vapour temperature leaving the superheater is controlled by a third P+I controller, TIC.

Figure 8.1 : Nitric Acid Plant Ammonia Vaporiser Control System



The ammonia flowrate leaving the superheater is controlled by the ammonia:air ratio controller, FrRC which regulates the flow of ammonia.

It can be seen that a throttling of the ammonia flowrate by FrRC causes the pressure in the upstream system to increase. This in turn causes PIC to reduce the cooling water fed to the vaporiser. The reduction in cooling water flow causes a reduction in vaporisation and therefore an increase in liquid level in the vaporiser. The increase in liquid level causes LIC to reduce the liquid ammonia feed. In this way the four controllers interact with each other, a change at one leading to compensation by the others and therefore the trainee will discover that very careful operation is required. The ammonia vaporiser plays a key role in the Nitric Acid Process and the consequences of mis-operation are both dangerous and very expensive. In particular, mis-operation can lead to more extensive damage in downstream equipment.

The structure of the instructional programme is shown in Figure 8.2(B12). The programme is comprised of seven modules. The first five modules introduce the four control loops so that the trainee can identify the instrument on the plant control panel and relate recorded information and control action to the effect on the actual process. The remaining two modules feature a simulation of the actual operation and allow the trainee to investigate the operation of the system and practise diagnosing typical process faults.

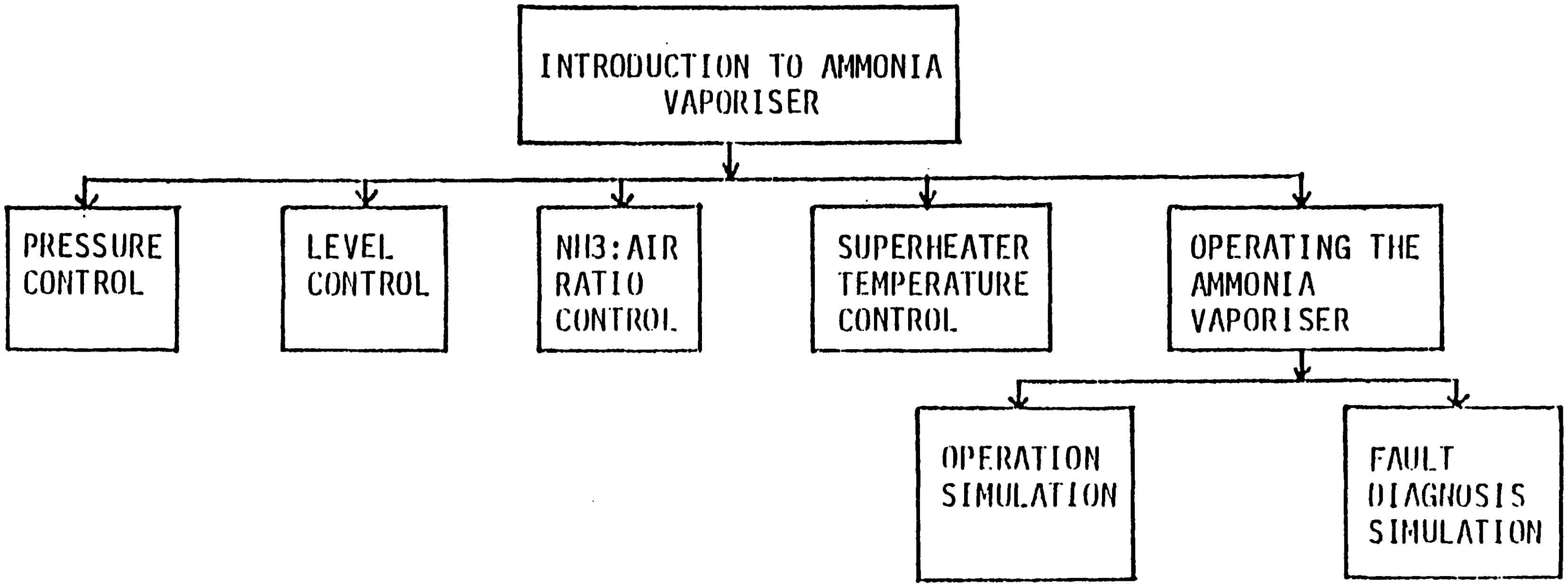


Figure 8.2 : Nitric Acid Plant Ammonia Vaporiser Control Instructional Module Structure

The objectives of the simulation are :-

(a) To demonstrate the operation of the Nitric Acid Plant ammonia vaporiser control system.

(b) To demonstrate the effect of some typical process faults and disturbances on the Nitric Acid Plant ammonia vaporiser.

(c) To give practice in fault diagnosis.

The structure of the two simulation modules is as given in Figure 6.1. The 'USE' language code for the lessons 'nit5bb6' and 'nit5bb6a' which make up the ammonia vaporiser control program are given in Appendix 3.8. A description of the program as seen by the trainee is given in section 8.2.3 and a comparison with actual plant data in section 8.2.4. First of all a description of the equations which model the operation of the system will be described in the next section 8.2.2.

8.2.2 Mathematical Model

The ammonia vaporiser is essentially a vertical shell and tube heat exchanger with ammonia on the shellside and cooling water on the tubeside. A detailed mathematical model of a heat exchanger involves the derivation of a set of partial differential equations to take account of the spatial variations of the parameters within the exchanger. However, a greatly simplified model which shows the essential responses of the vaporiser to changes in feed conditions and pressure is sufficient to achieve the objectives of the desired training. Therefore, the vaporiser will be represented by a lumped parameter approximation. This takes the form of a continuously stirred tank surrounded by a water jacket. The model assumes that the ammonia liquid and vapour are in thermodynamic equilibrium at a set vaporisation temperature. The liquid and vapour phases are well mixed so that temperature is constant throughout each phase. It does not take into account the spatial variations in temperature within the vaporiser which could occur on the actual plant. It also assumes that the ammonia vapour exhibits ideal gas behaviour in the downstream equipment.

Considering the shellside, an ordinary differential equation can be written to describe the variation of the liquid ammonia volume, Vl with time, t :-

$$\frac{dVl}{dt} = \frac{Fl - Fe}{\rho l} \qquad \text{........(8.1)}$$

where Fl = liquid ammonia feed mass flowrate

Fe = rate of ammonia vaporisation

ρl = liquid ammonia density

The liquid ammonia feed flowrate can be calculated as follows :-

$$Fl = lCv * \sqrt{Pl - (Pv + (hl * \rho l * g))} \qquad \text{........(8.2)}$$

where P_l = liquid ammonia feed pressure

P_v = ammonia vapour pressure in downstream equipment

h_l = vaporiser liquid ammonia level $= \dfrac{V_l}{A_{vap}}$ ....(8.3)

A_{vap} = vaporiser cross-sectional area

g = gravitational constant

lC_v = liquid ammonia feed control valve discharge coefficient

The rate of ammonia vaporisation is dependent on the amount of heat transferred by the cooling water flowing through the tubeside. Since the flowrate of cooling water is high the dynamics of heat transfer can be ignored as follows :-

$$F_e = \frac{Q_{vap}}{H_{vap}} \qquad \text{........(8.4)}$$

where H_{vap} = latent heat of vaporisation of liquid ammonia

The vaporiser heat load is calculated as follows :-

$$Q_{vap} = UA * \frac{((T_v - T_1) + (T_v - T_2))}{2} \qquad \text{........(8.5)}$$

where UA = heat transfer rate coefficient

T_v = ammonia vapour temperature

T_1 = cooling water inlet temperature

T_2 = cooling water exit temperature

All temperatures are in absolute units.

Assuming an average overall heat transfer coefficient, the heat transfer rate coefficient, UA is only dependent on the level of liquid ammonia in the vaporiser as follows :-

$$UA = \frac{hl}{hlmax} * UAmax \qquad \text{........(8.6)}$$

where UAmax = maximum heat transfer rate coefficient

hlmax = maximum vaporiser liquid ammonia level

The cooling water exit temperature, T2 is calculated from the cooling water mass flowrates and temperatures and vaporiser heat load using :-

$$T2 = \frac{Qvap + W1 * Cpw * T1}{W2 * Cpw} \qquad \text{........(8.7)}$$

where Cpw = cooling water specific heat capacity

W1 = cooling water mass flowrate into vaporiser

W2 = cooling water mass flowrate exit vaporiser = W1

The cooling water inlet temperature is dependent on the cooling water fed from the main and the condensate collected from the ammonia superheater. Assuming that the specific heat capacity of the cooling water is constant, the inlet cooling water temperature can be calculated as follows :-

$$T1 = \frac{W5 * T5 + W4 * T4}{W1} \qquad \text{........(8.8)}$$

where $W4$ = mass flowrate of condensate from superheater

= S

S = mass flowrate of steam fed to superheater

$T4$ = temperature of condensate from superheater

$W5$ = mass flowrate of cooling water from main

$T5$ = temperature of cooling water from main

The mass flowrate of cooling water to the vaporiser is calculated as follows :-

$$W1 = W4 + W5 \qquad \text{........(8.9)}$$

The flowrate of cooling water fed from the main is dependent on the vaporiser pressure control valve :-

$$W5 = pCv * \sqrt{Pw} \qquad \text{.......(8.10)}$$

where Pw = cooling water main pressure

pCv = vaporiser pressure control valve discharge coefficient

The ammonia vapour temperature, Tv is dependent on the ammonia pressure in the downstream equipment. An Antoine relationship can be used as follows:-

$$Pv = \exp(A + B/Tv + C*Tv + D*\ln(Tv)) \qquad \text{.......(8.11)}$$

where A, B, C, D are constants.

Equation 8.11 can be solved for Tv given a value of Pv using Newtons method.

Assuming ideal gas behaviour, an ordinary differential equation can be written to describe the variation of pressure in the vaporiser, Pv with time, t as follows :-

$$\frac{dPv}{dt} = \frac{(Fe - Fv)}{MW} * \frac{R*Tv}{(Vv + Ve)} \qquad ....(8.12)$$

where Fv = ammonia vapour flowrate in downstream equipment

R = gas constant

MW = molecular weight of ammonia

Vv = volume of vapour in vaporiser

Ve = volume of vapour in downstream equipment

The volume of vapour in the downstream equipment is assumed to be constant. The volume of vapour in the vaporiser is determined as follows :-

$$Vv = Vm - Vl \qquad ....(8.13)$$

where Vm = total volume of vaporiser shell

Vl = volume of liquid ammonia in vaporiser

The flowrate of vapour in the downstream equipment is dependent on the air:ammonia ratio control valve :-

$$Fv = rCv * \sqrt{Pv} \qquad ....(8.14)$$

where rCv = air:ammonia ratio control valve discharge coefficient

Some liquid is always carried over from the vaporiser with the ammonia vapour and to account for this a function was estimated empirically from plant experience :-

$$x = \frac{(hl - 1.7)^2}{10} \qquad \text{.......(8.15)}$$

where x = fraction liquid in vapour stream

Some of the liquid carried over from the vaporiser is vaporised in the superheater. The dynamic response of the superheater is much faster than that of the vaporiser. Since we are mainly concerned with the operation of the ammonia vaporiser the superheater dynamics will be assumed to be instantaneous. Therefore the superheater can be represented by steady-state relationships as follows :-

$$q = S * Hsteam \qquad \text{.......(8.16)}$$

where Hsteam = latent heat of saturated steam @ 35 psig

q = initial estimate of superheater heat load

Assuming that the heat load, q is first utilised in vaporising any remaining liquid, the actual superheating supplied to the ammonia vapour, qs is :-

$$qs = q - x*Fv*Hvap \qquad \text{.......(8.17)}$$

If qs is negative then some liquid ammonia will remain in the ammonia vapour and the temperature of the vapour leaving the superheater, Tve will be equal to the temperature exit the vaporiser, Tv. The liquid fraction remaining in the ammonia vapour is calculated as follows :-

$$y = \frac{(x*Fv - q/Hvap)}{Fv} \qquad ....(8.18)$$

where y = liquid fraction remaining in ammonia vapour after superheater.

If qs is positive then the liquid carry over is fully vaporised and the temperature of the ammonia vapour exit the superheater, Tve is calculated from an enthalpy balance as follows :-

$$Hve = Hv + qs \qquad ....(8.19)$$

where Hv = enthalpy of ammonia vapour and liquid fed to superheater

Hve = enthalpy of ammonia vapour leaving superheater

The routine 'suptemp' given in lesson 'nit5bb6' in Appendix 3.8 then carries out an iterative calculation to determine the temperature of the ammonia vapour exit the superheater, Tve which corresponds to the enthalpy, Hve.

The air:ammonia ratio is based on the amount of ammonia vapour present and therefore the ratio is calculated as follows :-

$$ratio = \frac{(1-y)*Fv/\rho v*100}{Fa + (1-y)*Fv/\rho v} \qquad ....(8.20)$$

where Fa = Volumetric flowrate of air

ρv = Density of ammonia vapour

It will be seen later in section 8.2.4 that the animated mimic plant control panel which the trainee uses to operate the simulation requires that the temperature of the air/ammonia mixture and of the gauzes in the downstream nitric acid converters are displayed. An enthalpy balance is performed to determine the air/ammonia temperature exit the mixer, Tm. A simple correlation has been derived from plant experience which relates the air:ammonia ratio to the converter gauze temperature. This will be used since only an estimate of the gauze temperature is required as follows :-

$$Tg = Tm + 71*ratio \qquad ....(8.21)$$

where Tg = Nitric acid converter gauze temperature

These equations can then be solved using the algorithm shown in Figure 6.2 and described in section 6.4.2. Equations 8.2, 8.3, 8.4, 8.5, 8.6, 8.7, 8.8, 8.9, 8.10, 8.11, 8.13, 8.14, 8.15, 8.16, 8.17, 8.18, 8.19, 8.20 and 8.21 are the algebraic equations. Equations 8.1 and 8.12 are the time dependent derivatives. The integration is carried out using the 'intin' and 'intde' routines described in Appendix 2.

The four control loops are modelled using the 'PIcontr' routine. The discharge coefficients of the four associated control valves are modelled using the 'valve' routine. These routines are also described in Appendix 2.

The program includes 6 typical process faults and disturbances which occur on the ICI Severnside Nitric Acid Plant Ammonia Vaporiser. These are listed in Table 8.1 below. The faults are simulated by 'switching' various parts of the model on and off and by changing the values of some parameters as described for the steam heated heat exchanger control program in section 7.2.1.3 of Chapter 7.

The 'USE' language code for the simulation calculations are given in section 'simcalcs' and for the fault simulation in section 'fault' of the lesson 'nit5bb6' given in Appendix 3.8.

Table 8.1 Nitric Acid Plant Ammonia Vaporiser Control Process Faults and Disturbances.

Process Faults And Disturbances

1. Drop in liquid ammonia feed pressure
2. Fouling of vaporiser heat transfer surface with oil
3. Excessive liquid ammonia carry-over from vaporiser
4. Increase in plant air flowrate
5. Drop in steam pressure to superheater
6. Fouling of vaporiser offtake line at the superheater inlet

8.2.3 The Program as Seen by the Trainee

A sample of the screen displays seen by the trainee are given in Figures 8.3 to 8.11. Figure 8.3 shows an example display from the 'introduction' module. This module picks out the control panel instruments which are associated with the ammonia vaporisation system. Figure 8.4 shows an example display from the module on the air:ammonia ratio controller. This module describes the operation of the controller and its effect on the process operations.

Figures 8.5 to 8.11 are samples of the screen displays from the last two modules which feature the simulation of the actual operation. Figure 8.5 is one of the screen displays which introduce the trainee to the operation of the whole system.

Figure 8.6 shows the mimic plant control panel display used by the trainee to operate the simulation. Animated representations of the actual plant instrumentation are used. The relative positions of the individual instruments are retained on the condensed display. The mimic panel consists of two strip-chart recorder-controllers, one for the air:ammonia ratio and one for the ammonia vapour pressure. The controller signals to the respective control valves are shown above the charts in the normal way.

Figure 8.3 : Nitric Acid Plant Ammonia Vaporiser Control
Introduction Module

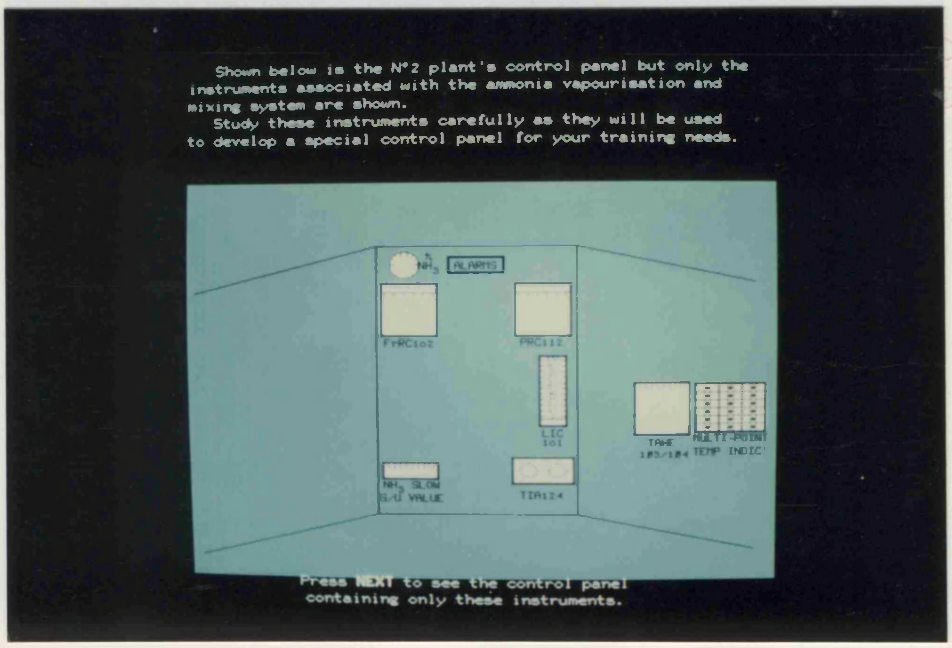


Figure 8.4 : Nitric Acid Plant Ammonia Vaporiser Control
Air:Ammonia Ratio Control Module

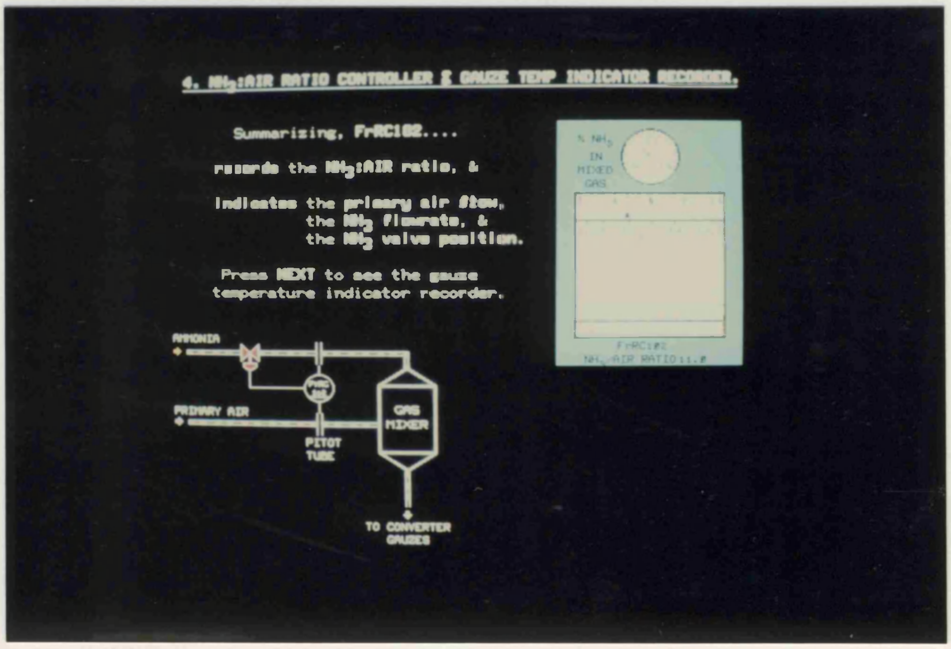


Figure 8.5 : Nitric Acid Plant Ammonia Vaporiser Control Simulation Introduction

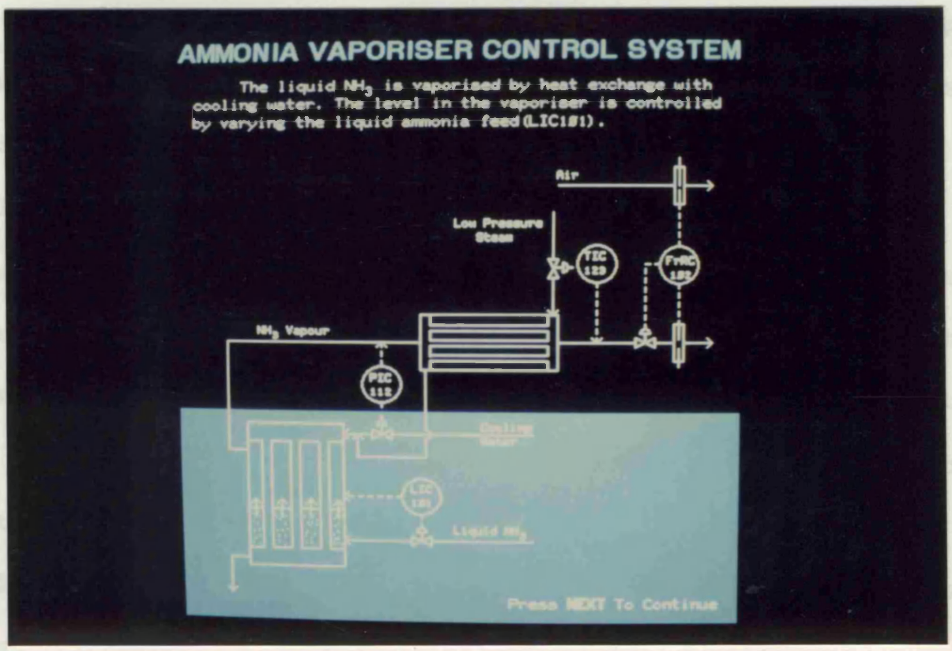
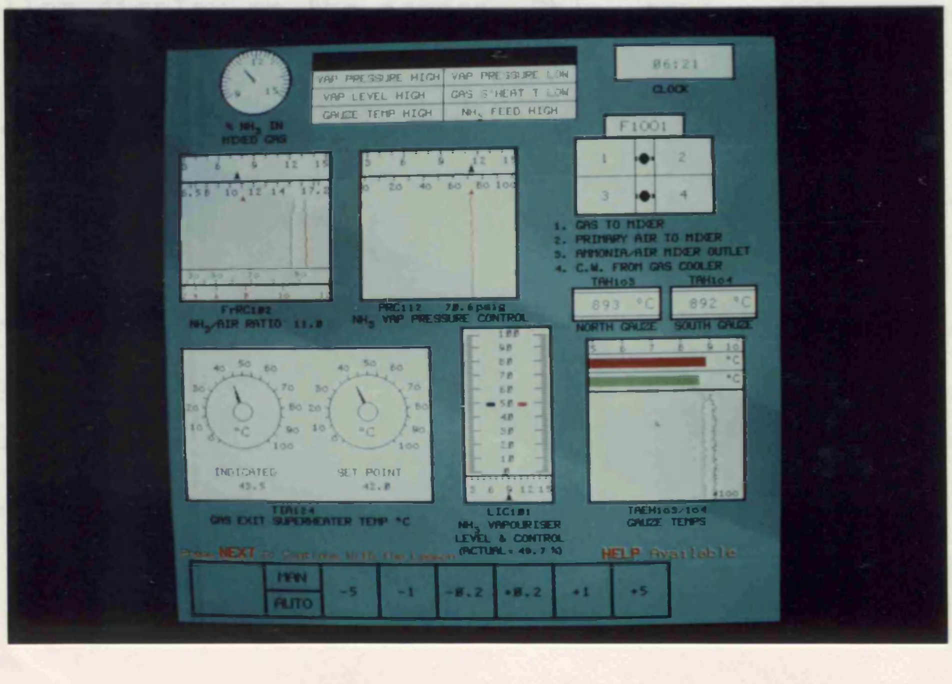


Figure 8.6 : Nitric Acid Plant Ammonia Vaporiser Control Mimic Plant Control Panel



The panel also features a West Gardian temperature indicator-alarm for the superheater exit temperature and a multi-point temperature indicator for the other plant temperatures such as cooling water and air/ammonia vapour mixture. The vaporiser liquid ammonia level is displayed on a level indicator-controller and the nitric acid converter gauze temperatures on a further strip-chart recorder. At the top of the panel there is a representation of part of the plant alarm panel. This includes all the alarms directly associated with the ammonia vapourisation system. These will flash and anunciate in the normal way when particular values go out of bounds.

A series of touch panel boxes is displayed at the bottom of the screen. In order to change the setpoint of one of the controllers, the trainee has to first of all select which controller he wishes to change by touching the appropriate controller display on the screen. Then, he can select the magnitude of the desired change by touching one of the option boxes which will be displayed for that particular controller. He can also change the mode of operation of the controller from automatic to manual. In which case he can then open and close the particular control valve directly using the same procedure as for the setpoint. The trainee can obtain guidance on the operating procedure at any time by pressing the 'help' key.

The trainee is allowed to 'play' with the simulation at his own pace. Figure 8.7 shows the effect of a setpoint change in the air:ammonia ratio. In this way, the trainee can investigate the response of the system to various setpoint and valve changes and so learn about the system by discovery.

When the trainee has become familiar with the operation of the system he can move on to the final module on common plant faults and fault diagnosis. The trainee is introduced to the possible faults and methods of detecting faults(eg Figure 8.8). He is then shown a particularly dangerous plant fault of liquid carry-over. The effect of the fault is described as in Figure 8.9.

Finally the trainee is allowed to operate the system and introduce faults entirely at his own pace. The example fault is included as one of six common process faults associated with the ammonia vaporisation system included in the program. These are selected at random when the trainee touches the box marked 'FAULT'. Figure 8.10 shows the effect of fouling of the vaporiser offtake line at the superheater inlet. The trainee is asked to attempt to diagnose the nature of the induced fault and to switch to the fault diagnosis display as shown in Figure 8.11 when he thinks he knows what it is. Figure 8.11 confirms that the correct answer is fault no 6. If the answer had been incorrect, then the program would have given him guidance as to where to look for the correct answer.

Figure 8.7 : Nitric Acid Plant Ammonia Vaporiser Control
Setpoint Change

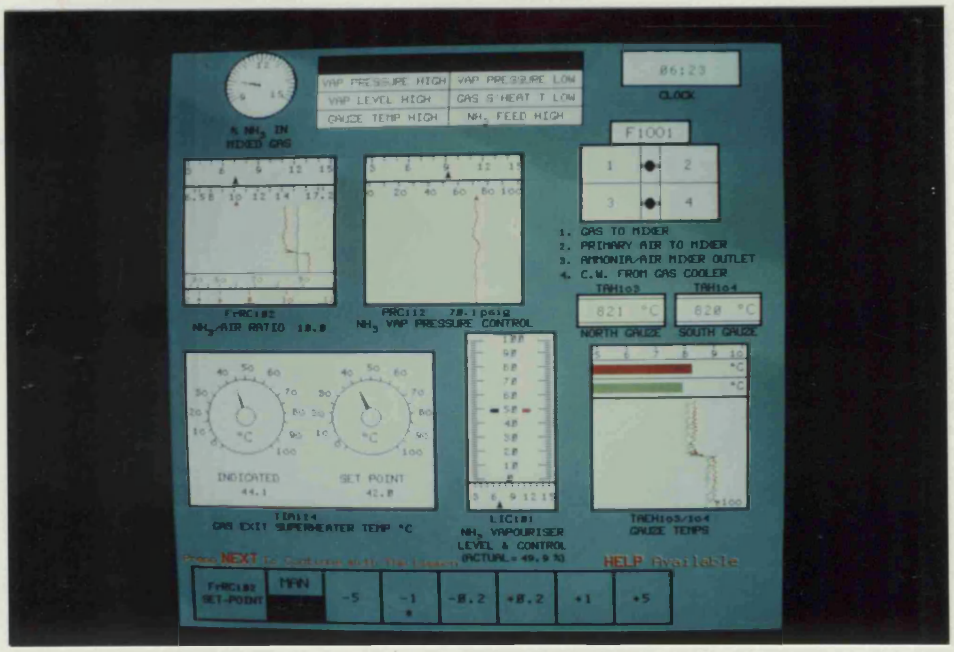


Figure 8.8 : Nitric Acid Plant Ammonia Vaporiser Control
Fault Diagnosis Introduction

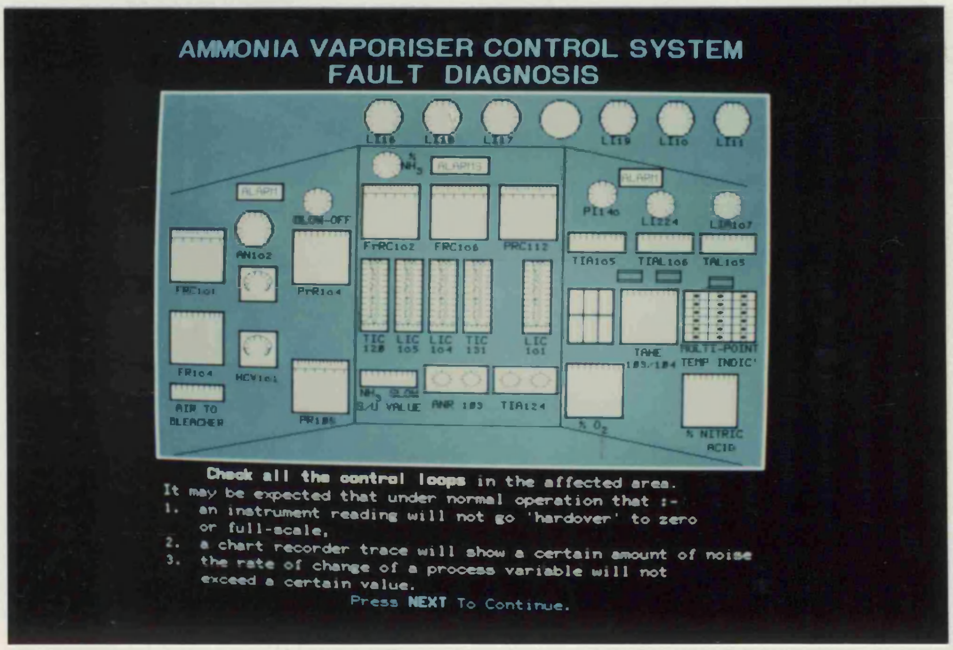


Figure 8.9 : Nitric Acid Plant Ammonia Vaporiser Control
Process Disturbance

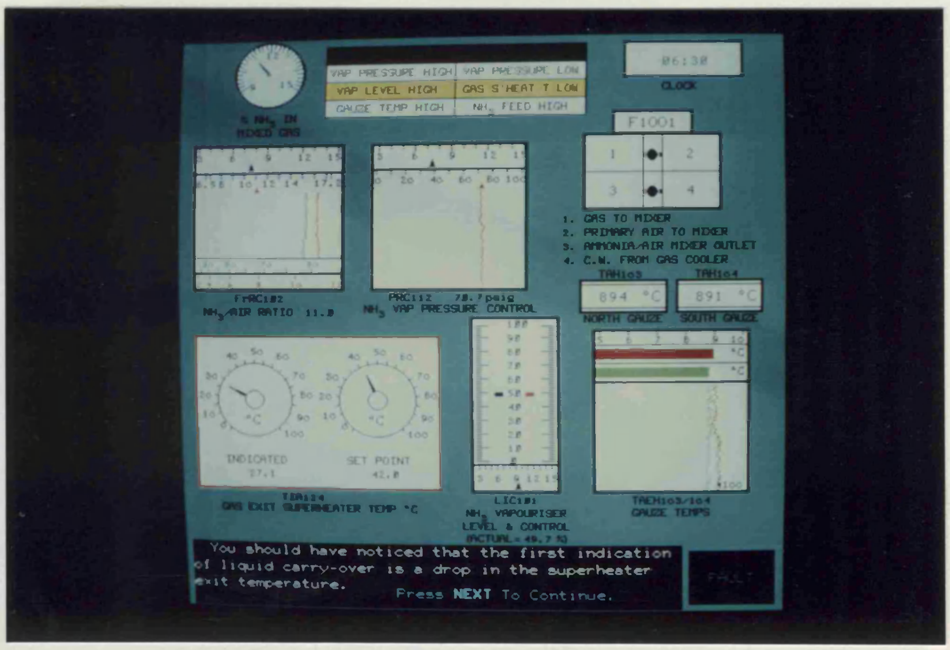
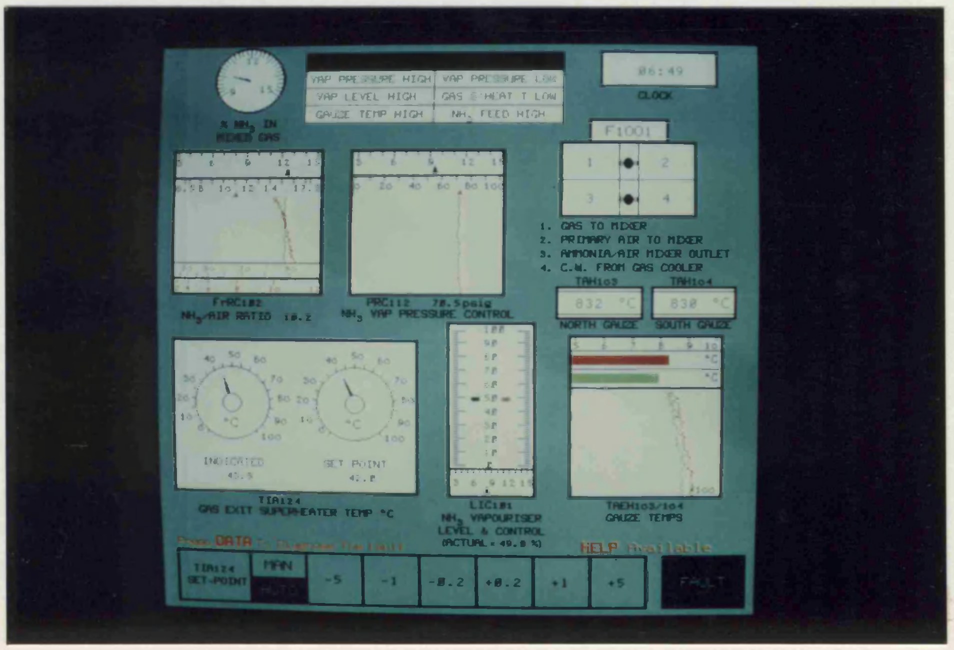


Figure 8.10 : Nitric Acid Plant Ammonia Vaporiser Control
Fault Simulation



Once the trainee has diagnosed the fault correctly he can return to the simulation either at the same point at which he left but with the fault removed so that he can see the effect of removing the fault or at normal steady-state conditions so that another fault can be introduced.

8.2.4 Comparison with Actual Plant Data

A comparison between the simulation and actual plant data is given in Table 8.2. Comparisons are given at four different air:ammonia ratios with the data drawn from plant record sheets. The data cover most of the parameters which are displayed on the animated mimic control panel display.

The accuracy of simulations used for training has been discussed in section 6.5 of Chapter 6. It was pointed out that differences between the simulation and the actual plant which do not affect the operator's judgement or do not result in an incorrect course of action have a negligible effect in the training environment. 'Critical' parameters which the trainee manipulates and observes directly should be fairly accurate. The American National Standard for Nuclear Power Plant Simulators states that 'critical' parameters should be within 2% of the actual plant readings. Similarly, 'non-critical' parameters which the trainee does not observe directly or are not displayed on the screen can be less accurate, for example 10% according to the American National Standard.

Table 8.2 Nitric Acid Plant Ammonia Vaporiser Control
Plant/Simulation Comparison

Table 8.2a Date: 27/2/86

	Plant	Simulation	% Error
Critical Parameters			
Air:Ammonia Ratio	11.8	11.8	0
Primary Air Flow(m3/hr)	54000	54000	0
Ammonia Vapour Flow(m3/hr)	7200	7225	0.3
Converter Gauze Temperatures(C)			
NORTH	880	889	0.9
SOUTH	880	886	0.7
Ammonia Vapour Pressure(psig)	69	69.2	0.3
Non-critical Parameters			
Primary Air Temperature(C)	128	128	0
Mixed Gas Temperature(C)	112	116.2	3.8
Cooling Water Temperature(C)	33	50	51.5
Ammonia Vapour Temperature(c)	59	72.2	22.4
Ammonia Vaporiser Temperature(C)	2	7.5	275.0

Table 8.2b Date: 24/4/86

	Plant	Simulation	% Error
Critical Parameters			
Air:Ammonia Ratio	11.5	11.5	0
Primary Air Flow(m3/hr)	74500	74500	0
Ammonia Vapour Flow(m3/hr)	9700	9686	0.1
Converter Gauze Temperatures(C)			
NORTH	880	881	0.1
SOUTH	880	880	0
Ammonia Vapour Pressure(psig)	70	70.6	0.9
Non-critical Parameters			
Primary Air Temperature(C)	149	149	0
Mixed Gas Temperature(C)	130	129.3	0.5
Cooling Water Temperature(C)	33	50	51.5
Ammonia Vapour Temperature(c)	59	56.4	4.4
Ammonia Vaporiser Temperature(C)	4	8	50.0

	Plant	Simulation	% Error

Table 8.2c Date: 19/3/86

Critical Parameters	Plant	Simulation	% Error
Air:Ammonia Ratio	11.3	11.3	0
Primary Air Flow(m3/hr)	80000	80000	0
Ammonia Vapour Flow(m3/hr)	10200	10193	0.1
Converter Gauze Temperatures(C)			
NORTH	875	868	0.8
SOUTH	875	866	1.0
Ammonia Vapour Pressure(psig)	75	74.8	0.3
Non-critical Parameters			
Primary Air Temperature(C)	147	147	0
Mixed Gas Temperature(C)	128	128.9	0.7
Cooling Water Temperature(C)	36	50	38.9
Ammonia Vapour Temperature(c)	56	53.9	3.8
Ammonia Vaporiser Temperature(C)	10	9.4	6.0

Table 8.2d Date: 30/6/86

Critical Parameters	Plant	Simulation	% Error
Air:Ammonia Ratio	11.1	11.1	0
Primary Air Flow(m3/hr)	83000	83000	0
Ammonia Vapour Flow(m3/hr)	10400	10362	0.4
Converter Gauze Temperatures(C)			
NORTH	878	861	1.9
SOUTH	865	859	0.7
Ammonia Vapour Pressure(psig)	76	75.8	0.3
Non-critical Parameters			
Primary Air Temperature(C)	157	157	0
Mixed Gas Temperature(C)	137	136	0.7
Cooling Water Temperature(C)	32	50	56.0
Ammonia Vapour Temperature(c)	60	53.5	10.8
Ammonia Vaporiser Temperature(C)	8	9.6	20.0

Examining the data given in Table 8.2 it can be seen that the 'critical' parameters are within the 2% criterion for all the four air:ammonia ratios. The accuracy of the 'non-critical' parameters varies widely but with the exception of the cooling water temperature and the ammonia vaporiser temperature the accuracy is generally within the 10% criterion for all the four air:ammonia ratios. The cooling water temperature is consistently 40-50% inaccurate. This could have been reduced by 'tuning' the heat transfer rate coefficient, UA. However, since the UA value used is comparable to that expected by the plant's engineers and also plant personnel stated that they very rarely checked the cooling water temperature, UA was left untuned.

The value of the plant ammonia vaporiser temperature varies widely and plant personnel did not have much confidence in the control panel reading. The simulation value of temperature corresponds to the saturation value at vaporisation pressure whereas the plant value does not. The plant ammonia vaporiser temperature is measured by a thermocouple contained in a thermowell. It can be seen from the faults listed in Table 8.1 that fouling is a particular problem on the plant. Therefore it is quite likely that the thermowell will also become fouled. This could greatly affect the plant reading and therefore it is probably reasonable to assume that the value calculated by the simulation is closer to the true plant value.

It has been stated in section 6.5 of Chapter 6 that for training purposes, the transients of the simulation need only be qualitatively correct. The simulated transients should not violate physical laws of nature and they should be accurate in direction and sequence of occurence. The best people to quantitatively evaluate the accuracy of the transient responses and the operational fidelity in general are the experienced senior control room operators and plant supervisors. Figure A4.15 in Appendix 4 shows that 17% of ICI Severnside's Nitric Acid Plant operators who responded to the questionnaire thought that the simulation response was good when compared to the actual plant and 67% thought it was 'ok'. Only 16% thought that the simulation's response was bad.

8.2.5 Discussion

This program was well received by plant personnel at ICI's Severnside Works. Figure A4.11 in Appendix 4 shows that 53% of those who had seen the program considered it to be very useful and the remaining 47% considered it to be useful. In addition all of the Nitric Acid Plant personnel who had seen the program considered it to be either very useful or useful.

However, Figure A4.16 in Appendix 4 shows that 33% of the Nitric Acid Plant Personnel who responded to the questionnaire considered that the Ammonia Vaporiser Control simulation had only improved their knowledge of the plant a little. The remaining 67% thought it hadn't improved their knowledge at all. This could be due to the fact that the existing plant personnel have been working on that plant for a number of years and therfore are already very experienced in the plant's operation. The real benefit of the training package will come when new operators are being trained on the plant. This is borne out by one new operator who has been through the course and considered it to be very useful in his initial training about the Ammonia Vaporiser Control system.

8.3 Ammonia Plant Make Gas Boilers Control

8.3.1 Introduction

This program simulates the operation of the Make Gas Boilers control system shown in Figure 8.12. It consists of two shell and tube heat exchangers which raise steam by heat exchange with process gas from the Ammonia Plant Secondary Reformer. The temperature exit the Make Gas Boilers has to be controlled so that efficient conversion of carbon monoxide to carbon dioxide takes place in the downstream Shift Converter.

The Shift Converter inlet temperature is controlled by bypassing some of the hot process gas around the second Make Gas Boiler as shown in Figure 8.12. The process gas which passes through the second Make Gas Boiler is cooled by raising steam. It is mixed at the outlet with the hot gas bypassed around the boiler.

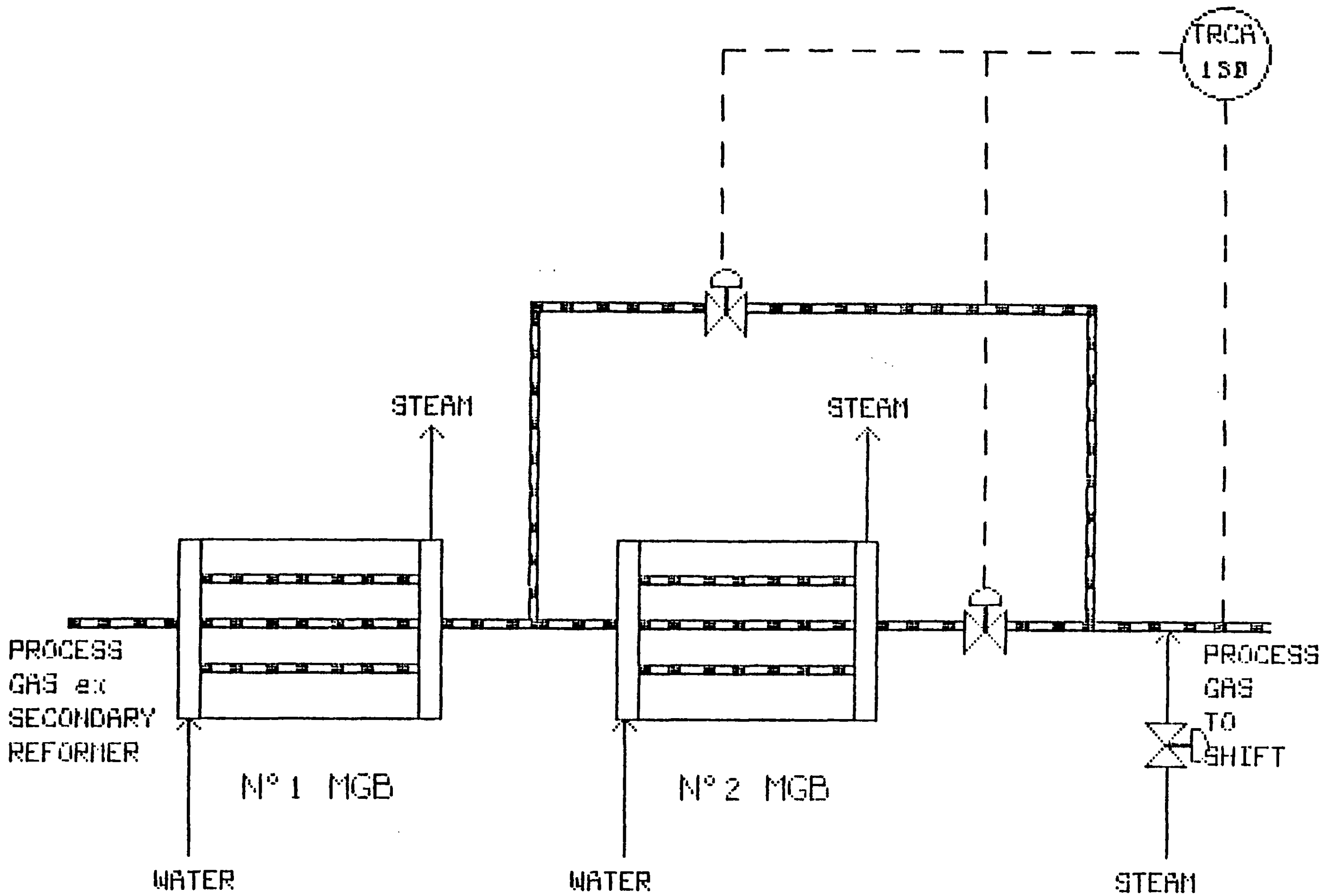


Figure 8.12 : Ammonia Plant Make Gas Boilers Control System

The Shift Converter inlet temperature is controlled by a proportional + integral split range controller, TRCA130. This increases and decreases the amount of hot gas bypassed around the boiler so that the Shift Converter inlet temperature is maintained at a steady value.

The split range controller, TRCA130 works by opening the bypass valve over the first half of its output range, 0-50%, and closing the inline valve over the second half of its range 50-100%. The bypass flowrate is increased by first of all opening the bypass valve until it is fully open at 50% and then further increases are achieved by restricting the flow through the second Make Gas Boiler which in turn forces more flow around the bypass.

It was found that the operators at ICI's Severnside Works had great difficulty in comprehending the operation of the system and therefore a training simulation package was developed. The objectives of the package are :-

(a) To enable plant personnel to be able to identify the location of the instruments associated with the Make Gas Boilers on the plant control panel.

(b) To demonstrate the operation of the Make Gas Boilers bypass controller, TRCA130

(c) To demonstrate the operation of the Make Gas Boilers and how they affect the downstream process units.

The structure of the program is as given in Figure 6.1. The program has a comprehensive introduction which describes the location of the instruments on the control panel and the operation of the split range controller, TRCA130. Then, the trainee is allowed to 'play' with the simulation and learn about the operation of the system by discovery. He is able to operate the system from animated mimic of the actual plant control room instrumentation. He can operate the controller in automatic or manual mode and observe the systems response on the screen display.

The 'USE' language code for the lessons 'mgbsim' and 'mgbsim1' which make up the Make Gas Boilers Control program are given in Appendix 3.9. A brief description of the program as seen by the user is given in section 8.3.3 and a comparison with actual plant data is given in section 8.3.4. First of all, a description of the equations which model the action of the control system will be given in the next section 8.3.2.

8.3.2 Mathematical Model

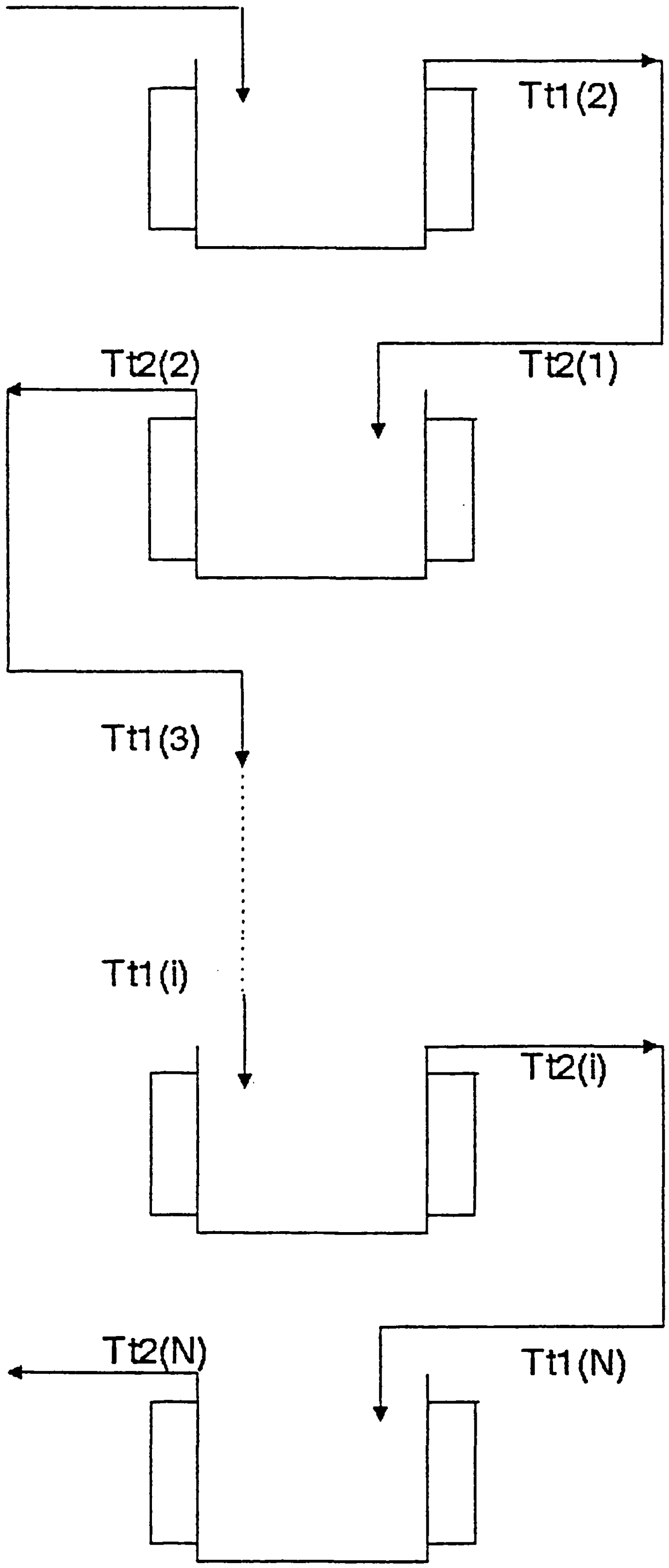
The two Make Gas Boilers can be considered to be co-current heat exchangers with steam being produced on the shellside by heat exchange with the hot process gas. The typical composition of the process gas exit the Ammonia Plant Secondary Reformer is given in Table 8.3.

Table 8.3 Ammonmia Plant Make Gas Boilers Control
Process Gas Inlet Composition

Carbon Monoxide	7.6 %
Carbon Dioxide	5.71 %
Hydrogen	38.99 %
Methane	0.37 %
Steam	34.56 %
Nitrogen	12.76 %

Therefore, a model can be developed which is similar to those described in section 7.2 of Chapter 7. Each Boiler can be represented by a series of lumped parameter approximations. These approximations take the form of continuous stirred tanks surrounded by steam jackets as shown in Figure 8.13. A sufficient number of lumped parameter approximations are used for each Make Gas Boiler so that the exit temperature from each boiler matches that given by plant data to a sufficient degree of accuracy.

Figure 8.13 : Stirred Tanks with Steam Jackets Model



Considering the ith lumped parameter approximation for either of the Make Gas Boilers :-

$$\rho t * Vt * Cpt(i) * \frac{dTt2(i)}{dt} = Hin(i) - Hout(i) + q(i) \qquad ....(8.22)$$

where ρt = tubeside vapour density

Vt = tubeside incremental volume

Cpt(i) = tubeside incremental vapour specific heat capacity

Tt2(i) = tubeside incremantal vapour exit temperature

Hin(i) = tubeside incremental vapour inlet enthalpy calculated at Tt1(i)

Tt1(i) = tubeside incremental vapour inlet temperature

Hout(i) = tubeside incremental vapour exit enthalpy calculated at Tt2(i)

q(i) = incremental heat transfer rate

The incremental vapour enthalpy and specific heat capacity are calculated for the composition given in Table 8.3 using correlations given in routine 'enth' in lesson 'mgbsim' in Appendix 3.9. An average temperature between adjacent increments is used to determine the inlet enthalpy in each case. The vapour density is assumed to be approximately constant throughout both Make Gas Boilers.

The heat transfer rate, q(i) is determined as follows assuming that the barrier between the shell and tube sides has negligible heat capacity :-

$$q(i) = U * A * deltaT(i) \qquad ....(8.23)$$

where U = overall heat transfer coefficient for that particular Make Gas Boiler

A = incremental heat transfer area

deltaT(i) = incremental log mean temperature difference

The overall heat transfer coefficient, U is dependent on the process gas flowrate through the particular boiler as follows :-

$$U = coeff * (ftot)^{0.8} \qquad ....(8.24)$$

where ftot = total tubeside vapour molar flowrate

coeff = constant

The incremental log mean temperature difference, deltaT(i) is calculated as follows :-

$$deltaT(i) = \frac{(Ts - Tt1(i)) - (Ts - Tt2(i))}{\ln((Ts - Tt1(i))/(Ts - Tt2(i)))} \qquad ....(8.25)$$

where Ts = saturated steam temperature in the particular Make Gas Boiler

The quantity (Ts - Tt1(i))/(Ts - Tt2(i)) is monitored as before to ensure that it does not become greater than 10^{15} or less than 10^{-13} as this causes the number range of the Regency microcomputer to be exceeded. This can occur as the incremental tudeside exit temperature approaches the saturated steam temperature and also if there is a sudden increase in the incremental tubeside inlet temperature. In such situations, the quantity is set to the maximum or minimum possible.

An iterative solution of the incremental heat balance equations is required since the incremental heat load, q(i) is required to calculate the exit temperatures from each increment but this is not known until the exit temperatures have been calculated. Therefore, initially the heat load is guessed and the exit temperature calculated. The heat load is then recalculated using the calculated exit temperature . The two heat loads are then compared and if the two values are not within 0.5% of each other then the guessed value of heat load is updated and the calculations repeated. The Wegstein convergence method was found to be the most robust convergence routine for use with the program, bearing in mind that the model has to withstand large deviations in parameters. The routine used, 'converg2' which employs the Wegstein method is described in the 'simpac' manual in Appendix 2.

The total flow through the Make Gas Boilers is fixed in the simulation. The algorithm described above is used to calculate the temperatures throughout the first Make Gas Boiler. Then the bypass flowrate around the second

Make Gas Boiler is calculated using the ratio of opening of the two control valves which make up the split range controller as follows :-

$$fbp = \frac{bfCv}{(bfCv + ifCv)} * ftot \qquad ....(8.26)$$

where bfCv = bypass flow control valve discharge coefficient

ifCv = inline flow control valve discharge coefficient

fbp = bypass vapour molar flowrate

The inline vapour flowrate is then calculated as follows :-

$$fint = ftot - fbp \qquad ....(8.27)$$

The heat balance algorithm is then used once more to calculate the temperatures throughout the second Make Gas Boiler. The bypass flow is added back to the flow through the second Make Gas Boiler together with process steam at the Make Gas Boilers exit :-

$$fout = fint + fbp + fsteam \qquad ....(8.28)$$

where fsteam = process steam flowrate added at the Make Gas Boilers exit

A further enthalpy balance is carried out using the routine 'enth' given in lesson 'mgbsim' in Appendix 3.9 to determine the inlet gas temperature to the Shift Converter.

It will be seen in the next section 8.3.3 that the animated mimic plant control panel which is used to operate the simulation requires that the temperature exit the shift converter is displayed. A steady-state routine was used to carry out the material and energy balances over the shift converter to determine a value for the exit temperature. This routine will be described in more detail in section 9.3.2.4 in Chapter 9.

The equations can be solved using the algorithm shown in Figure 6.2 and described in section 6.4.2. Equations 8.23, 8.24, 8.25, 8.26, 8.27 and 8.28 are the algebraic equations and equation 8.22 is the time dependent derivative. The integration is carried out using the 'intin' and 'intde' routines described in Appendix 2.

The split range controller, TRCA130 is modelled using the 'PIcontr' routine. Some additional logic was derived to model the split range action and this is given together with the rest of the simulation calculations in section 'simcalcs' of lesson 'mgbsim' in Appendix 3.9. The discharge coefficients of the two associated control valves were modelled using the 'valve' routine presented in the 'simpac' manual in Appendix 2.

8.3.3 The Program as Seen by the Trainee

A sample of the Ammonia Plant Make Gas Boilers Control program screen displays are given in Figures 8.14 to 8.16.

Figure 8.14 : Ammonia Plant Make Gas Boilers Control Title Screen

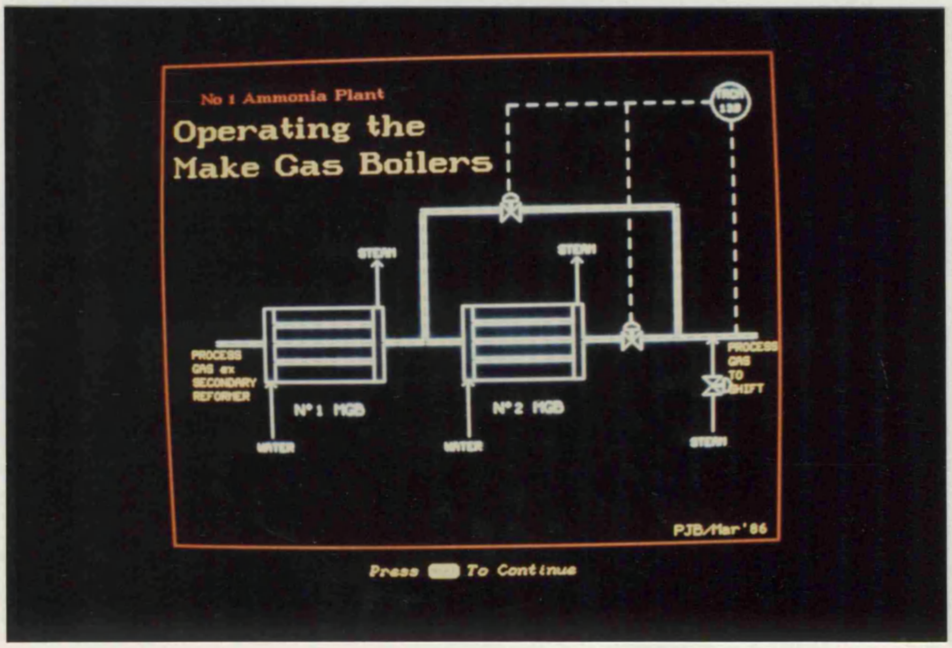


Figure 8.15 : Ammonia Plant Make Gas Boilers Control Introduction

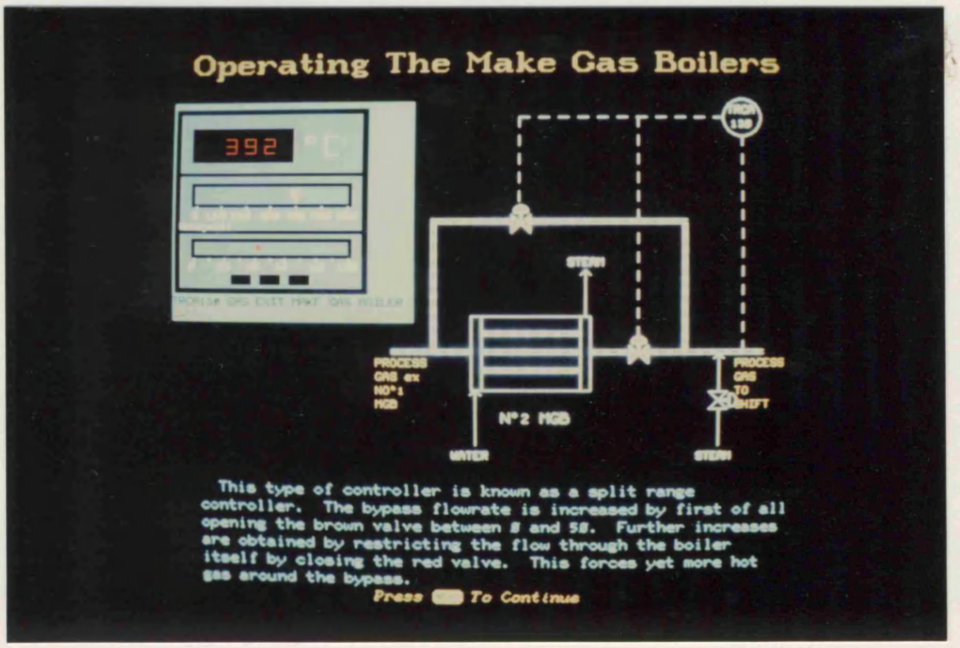


Figure 8.14 shows the opening display of the introduction. This introduces the trainee to the location of the instruments associated with the Make Gas Boilers on the control panel. Figure 8.15 shows one of the screen displays which describe the operation of the split range controller, TRCA130.

When the trainee has been through the introduction he is then allowed to operate the simulation using the mimic control panel display given in Figure 8.16. The animated display features a strip chart recorder for the process gas exit the Make Gas Boilers and Shift Converter temperatures and a digital/analogue display for the split range controller, TRCA130. The display also features a West Gardian temperature-indicator-alarm for the Secondary Reformer exit temperature and a multi-point temperature indicator for the other plant temperatures such as the process gas exit the first Make Gas Boiler. At the top of the panel there is a representation of part of the plant alarm panel. This includes all the alarms directly associated with the Make Gas Boilers. These will flash and anunciate in the normal way when particular values go out of bounds.

At the bottom of the display there is a number of touch panel boxes which allow the trainee to change the mode of operation, either automatic or manual of the split range controller. He can also change the controller setpoint operating in automatic mode and the valve position if operating in manual mode. The trainee can obtain help on operating the simulation at any time by pressing the 'help' key. Figure 8.15 shows the effect of increasing the Make Gas Boiler exit temperature setpoint. This results in an oscilatory increase in Make Gas exit temperature together with an associated rise in the Shift Converter temperature.

8.3.4 Discussion

A comparison between the simulation and actual plant data is given in Table 8.4. Using the accuracy criteria set in section 6.5 of Chapter 6 it can be seen that the 'critical' parameters are all within the required 2% error. The accuracy of the 'non-critical' parameters varies widely. In particular the composition exit the Shift Converter shows approximately a 30% discrepancy. However, the associated 'critical' Shift Converter exit temperature shows agreement within the 2% criteria and therefore since the trainee does not have access to the exit composition values they can be ignored.

Two Ammonia Plant Operators were asked their opinion of the transient response of the simulation. They agreed that the simulation's response was a good representation of the real plant. Unfortunately, however, the Ammonia Plant was shutdown and its personnel redeployed elsewhere before a formal evaluation of the usefulness and response of the training simulation could be carried out.

Table 8.4 Ammonia Plant Make Gas Boilers Control Plant/Simulation Comparison

	Plant	Simulation	% Error
Critical Parameters			
Temp. ex Secondary Reformer(C)	860	860	0
Temp. ex No 1 Make Gas Boiler(C)	560	550.6	1.7
Temp. inlet Shift Converter(C)	400	398.6	0.4
Temp. ex Shift Converter(C)	420	413.2	1.6
Temp. ex No 4 Feedwater Heater	188	188	0
Non-critical Parameters			
Comp. ex Secondary Reformer(%CH4)	0.3	0.37	23.3
Pres. ex Secondary Reformer(psig)	165	164.5	0.3
Steam fed inlet Shift Converter			
Flowrate(te/hr)	10	9.3	7.0
Temperature(C)	367	367.5	0
Pressure(psig)	300	300	0
Comp. ex Shift Converter(%CH4)	1.5	1.1	26.7
(%H2)	58.0	39.4	32.0
Pres. ex Shift Converter(psig)	160	160	0

Chapter 9 Specific Plant 'Cause And Effect' Simulations

9.1 Introduction

The selection of which mathematical modelling technique to use for training simulations depends on the objectives of the desired training. For example, if the dynamics play an important part in the simulation such as in teaching the operation of process control systems as in Chapters 7 and 8 then a dynamic model should be used. However, if the objective is just to demonstrate the inter-relationships between process variables then a model which represents these 'cause and effect' relationships can be used. This chapter presents two examples of 'cause and effect' simulations of actual plant systems which have been used for training plant personnel.

Two 'cause and effect' simulation approaches were described in section 6.4.3 of Chapter 6. The choice of which approach to use again depends on the quantity and quality of process data available. Since there are only limited process data available about the plants at ICI's Severnside Works, the 'steady-state snapshot' simulation approach will be used. This makes use of steady state material and energy balances to predict the plant inter-relationships.

A detailed description of the simulation of 'Ammonia Plant Ammonia Converter Operation' is given in the next section 9.2. This program was produced to demonstrate the effect of some modifications which were to be made to the Ammonia Plant. A brief description of the simulation of 'Ammonia Plant Reforming Section Operation' is given in section 9.3.

The training objectives of each example are specified in the relevant section. A comparison with actual plant data is given and opinions of the plant personnel of each simulation are presented. These opinions were obtained from a questionnaire, the results of which are presented in Appendix 4.

9.2 Ammonia Plant Ammonia Converter Operation

9.2.1 Introduction

This program simulates the operation of the ammonia converter which is part of the ammonia synthesis loop shown in Figure 9.1. The converter produces ammonia from synthesis gas according to the reaction :-

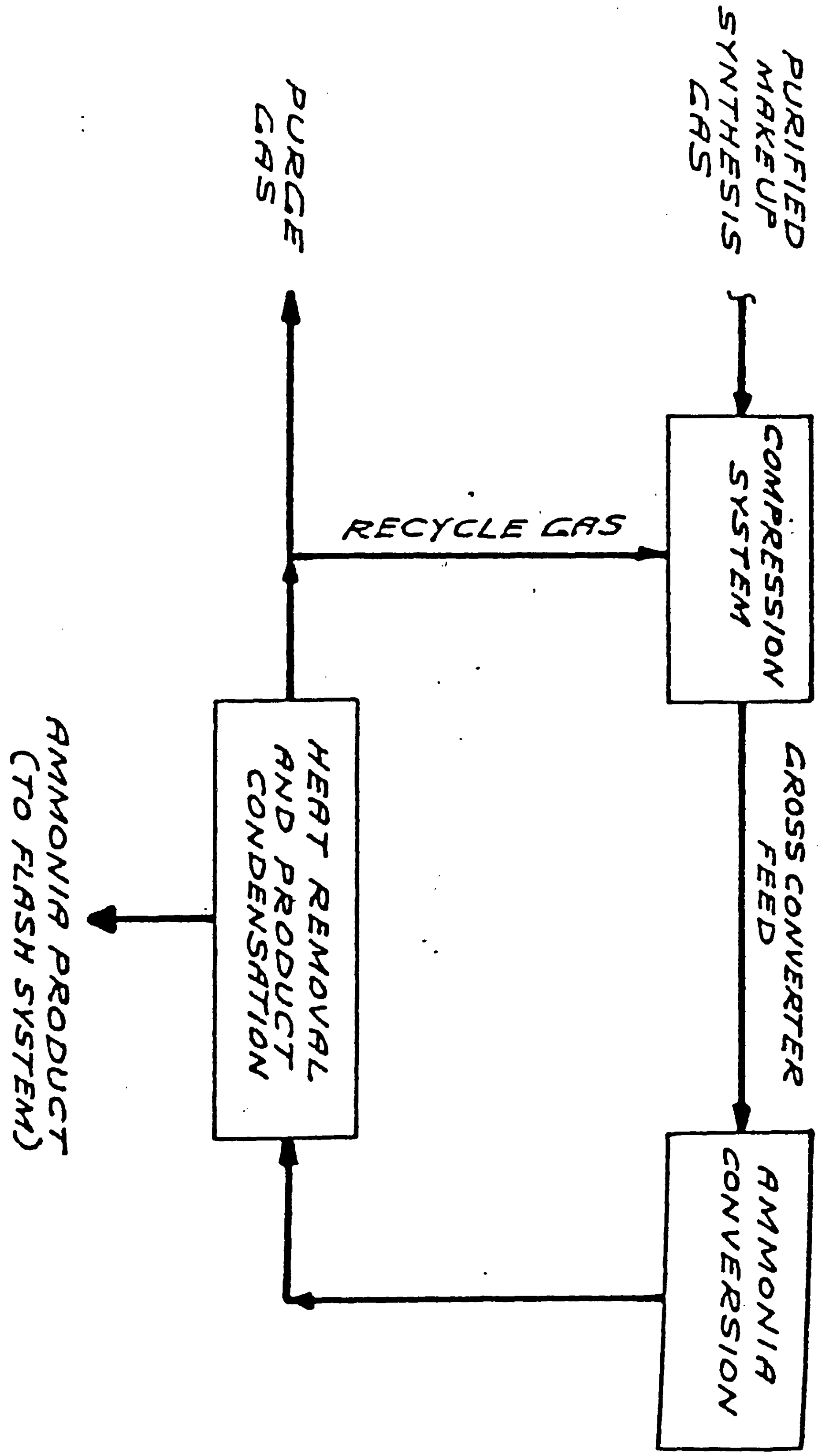
$$N_2 (g) + 3 H_2 (g) \rightleftharpoons 2 NH_3 (g) \qquad \text{........(9.1)}$$

The composition of the synthesis gas is given in Table 9.1.

Table 9.1 Ammonmia Plant Ammonia Converter Operation
Synthesis Gas Inlet Composition

1.	Hydrogen	64.25 %
2.	Nitrogen	21.42 %
3.	Ammonia	6.77 %
4.	Methane	3.83 %
5.	Argon	3.73 %

Figure 9.1 : Schematic Flow Diagram of the Ammonia Synthesis Process

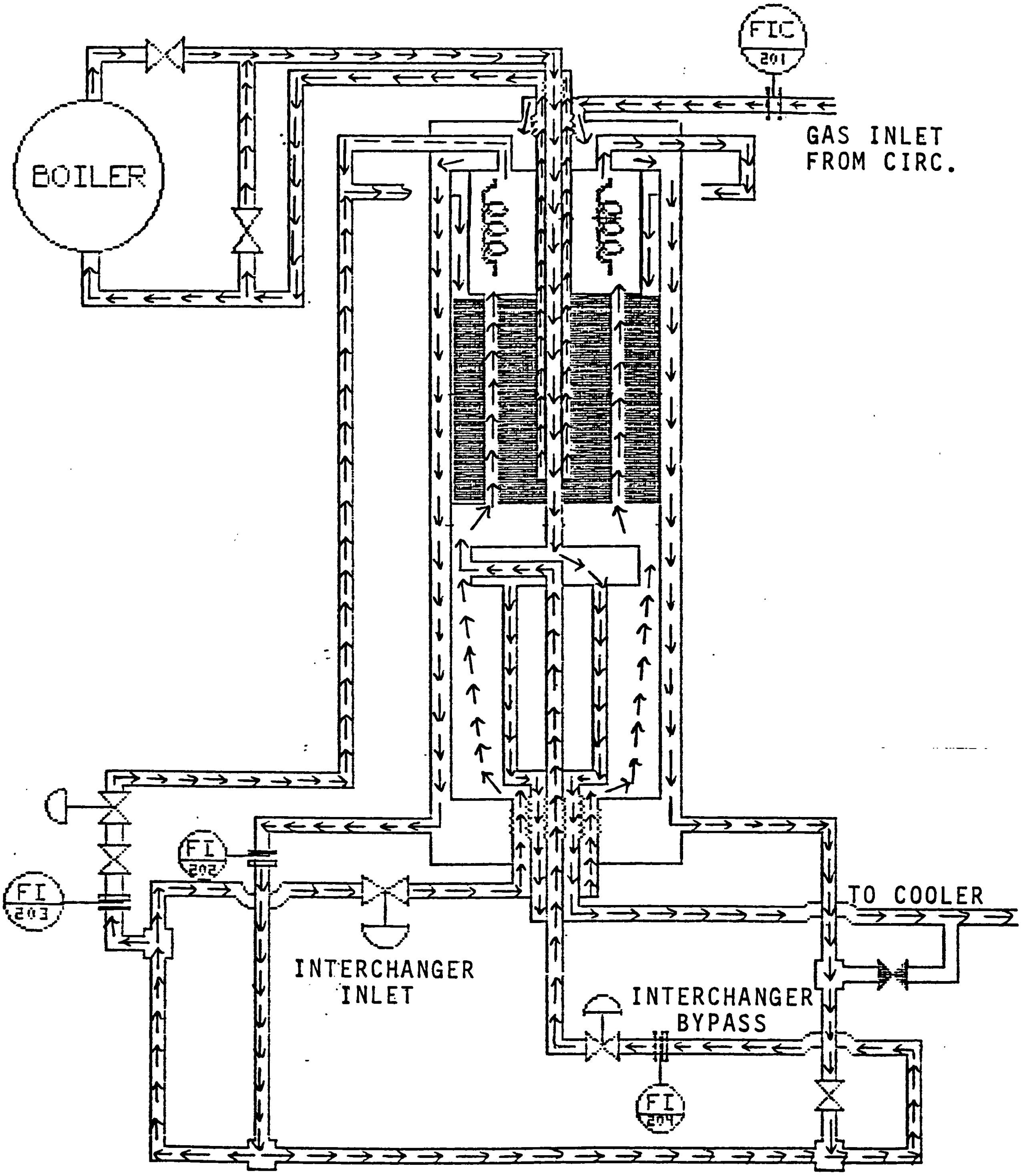


The ammonia converter is shown in Figure 9.2. It consists of a fixed bed catalytic reactor in which the incoming cold synthesis gas flows downward through the outer annular space to the base of the vessel. It then flows up through the shellside of the interchanger with the temperature of the gas exit the interchanger being controlled by opening and closing the interchanger inlet and bypass valves. The gas then passes up through the catalyst bed cooler tubes and then down through the catalyst bed itself. The inlet temperature of the gas to the bed can be controlled by bypassing some flow around both the interchanger and the bed tubeside pass. This is called the direct bypass and is mixed with the preheated synthesis gas at the inlet to the bed.

The hot reacted gas from the catalyst bed then flows up through a central annular space and passes through the converter boiler where saturated steam at 320psig is produced. The temperature exit the boiler can be controlled by bypassing flow around the boiler. The reacted gas then passes down through a centrally located pipe and through the tubeside of the interchanger and then away to a cooler.

All three bypass valves are controlled manually from the control room panel. The interchanger bypass and direct bypass can also be varied by throttling the interchanger inlet valve and hence forcing more flow through the two bypasses.

Figure 9.2 : Ammonia Converter



This program was developed to demonstrate the effect of some modifications which were to be made to the ammonia converter. It was proposed to plug one third of the catalyst bed cooler tubes to increase ammonia production by reducing the amount of heat transferred to the synthesis gas from the bed. This would mean that the interchanger bypass could be reduced and more heat recovered from the hot reacted gas in the interchanger. In addition, the gas leaving the catalyst bed cooler tubes is likely to be at a lower temperature and so less direct bypass would be required to control the peak temperature in the bed. As less gas is flowing around the direct bypass, more gas flows up through the cooler tubes. The increased flow up the tubes and the reduced heat transfer result in a change in the catalyst bed temperature profile. The temperature at the top and bottom of the bed should be hotter with a lower peak temperature. This should result in more of the catalyst working effectively and therefore increased ammonia production.

The program is split into three sections :-

(a) Description of modifications
(b) Effect of modifications on the plant parameters displayed on the control panel
(c) Simulation of the operation of the ammonia converter both before and after the modifications.

The latter two parts use a simulation of the operation of the ammonia converter. The effect of the modifications of the plant parameters displayed on the control panel is described and the simulation is used to show the effect on the bypass valve positions and on the temperature profile in the catalyst bed. The final part allows the trainee to 'play' with the simulation in either pre or post modification form to investigate the operation of the system and observe the consequences of his actions without the dangers of upsetting the real plant. The simulation is operated from an animated mimic of the actual plant control room instruments. The trainee can open and close the various valves just as he would on the real plant.

The objectives of the simulation are :-

(a) To demonstrate the effect of the modifications on the Ammonia Plant ammonia converter.

(b) To demonstrate the effects of the interchanger and direct bypasses on the catalyst bed temperature profile both before and after the modifications.

(c) To demonstrate the steady state operation of the Ammonia Plant ammonia converter system.

The structure of the two parts which use the simulation is shown in Figure 6.1. The 'USE' language code for the lessons 'amconsim', 'amconint' and 'amcoint2' which make up the ammonia converter operation program are given in Appendix 3.10.

A description of the program as seen by the trainee is given in section 9.2.3 and a comparison with actual plant data in section 9.2.4. First of all a description of the equations which model the operation of system will be described in the next section 9.2.2.

9.2.2 Mathematical Model

The ammonia converter is a very complicated system and therefore a dynamic model of the system would take some considerable time to develop. Since the objectives of the simulation only requires that the program demonstrates the 'cause and effect' relationships between the catalyst bed temperature profile and the various converter flowrates both before and after the modifications it was decided that the 'steady state snapshot' approach would be used.

Consider the flow diagram of the ammonia converter system shown in Figure 9.3. Taking the molar feed flowrate as f(1) at temperature T(1) and assuming that little heat transfer occurs as the gas passes down through the outer annular space then :-

$$f(2) = f(1) \qquad \text{........(9.2)}$$

$$T(2) = T(1) \qquad \text{........(9.3)}$$

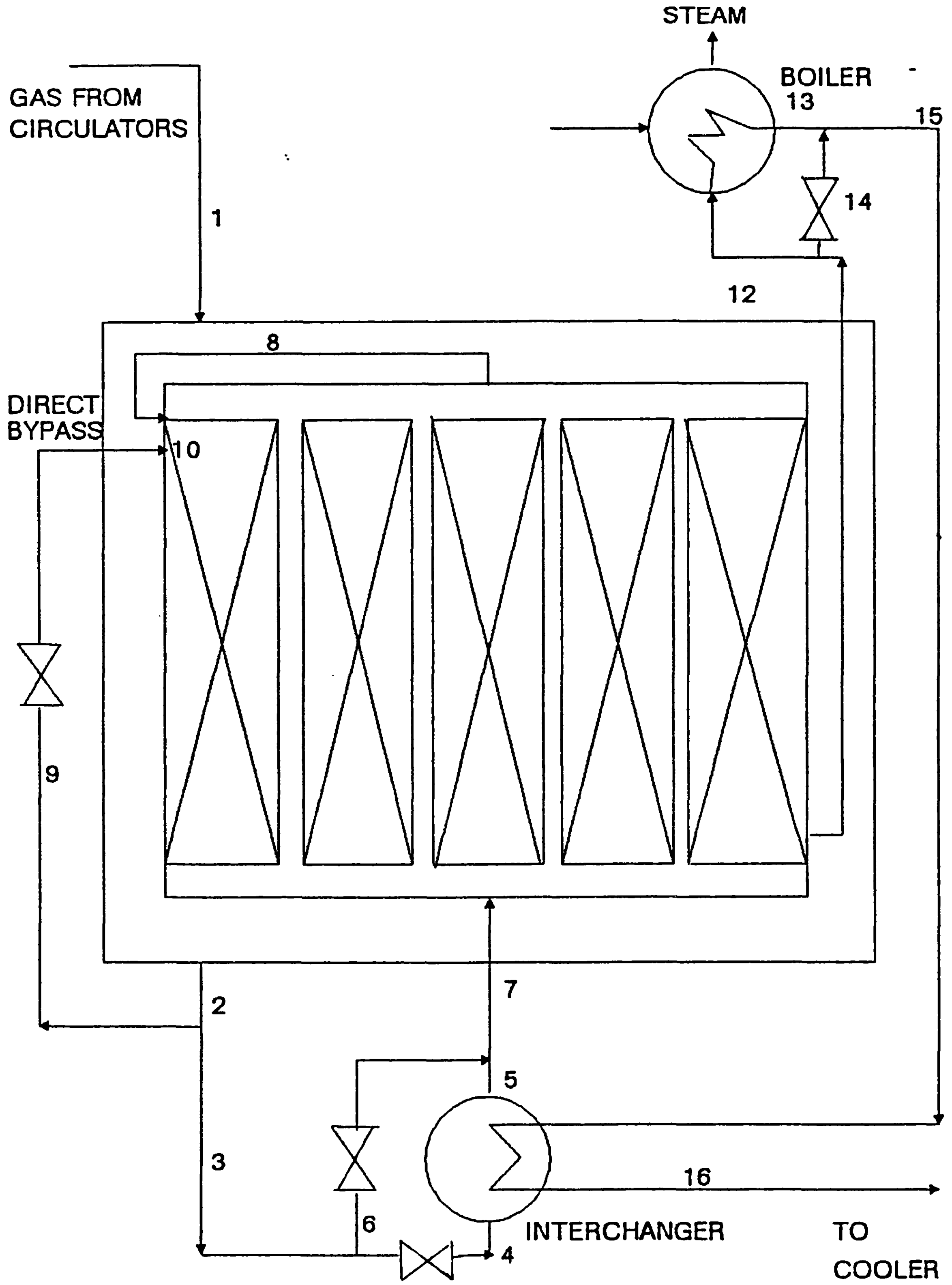
where f(i) = molar flowrate

T(i) = temperature

subscript 1 refers to synthesis gas feed conditions

subscript 2 refers to synthesis gas conditions exit the outer annular space

Figure 9.3 : Ammonia Converter Model



If the direct bypass molar flowrate is $f(9)$ then the flow and temperature after the direct bypass has been split are :-

$$f(3) = f(2) - f(9) \qquad \text{........(9.4)}$$

$$T(3) = T(9) = T(2) \qquad \text{........(9.5)}$$

where subscript 3 refers to the synthesis gas exit the direct bypass split

subscript 9 refers to the direct bypass

Similarly, the flow and temperature after the interchanger bypass has been split is :-

$$f(4) = f(3) - f(6) \qquad \text{........(9.6)}$$

$$T(4) = T(6) = T(3) \qquad \text{........(9.7)}$$

where subscript 4 refers to synthesis gas conditions exit the interchanger bypass split

subscript 6 refers to the interchanger bypass

The direct and interchanger bypass flows can be considered to be proportional to the interchanger inlet, interchanger bypass and direct bypass control valve positions as follows :-

$$f(6) = \frac{ibCv}{iCv + ibCv + dCv} * f(2) \qquad \text{........(9.8)}$$

$$f(9) = \frac{dbCv}{iCv + ibCv + dCv} * f(2) \qquad \text{........(9.9)}$$

where iCv = interchanger inlet valve discharge coefficient

ibCv = interchanger bypass valve discharge coefficient

dCv = direct bypass valve discharge coefficient

Assuming from plant experience that there is a 5C approach in temperature at the interchanger exit then :-

$$T(5) = T(15) - 5 \qquad ....(9.10)$$

$$f(5) = f(4) \qquad ....(9.11)$$

where subscript 5 refers to synthesis gas conditions exit the interchanger

subscript 15 refers to the reacted gas at the interchanger inlet

The interchanger heat load qI is therefore :-

$$qI = f(5) * Cpg * (T(5) - T(4)) \qquad ....(9.12)$$

where qI = interchanger heat load

Cpg = average specific heat coefficient

and the conditions of the reacted gas exit the interchanger become :-

$$f(16) = f(15) \qquad ....(9.13)$$

$$T(16) = \frac{f(15) * Cpg - qI}{f(16)*Cpg} \qquad ....(9.14)$$

where subscript 16 refers to the reacted gas at the interchanger exit

The interchanger bypass is then added back to the synthesis gas flow immediately after the interchanger as follows :-

$$f(7) = f(5) + f(6) \qquad ....(9.15)$$

where subscript 7 refers to the synthesis gas exit interchanger bypass addition

The temperature of the synthesis gas after the addition of the interchanger bypass is calculated assuming an average specific heat coefficient :-

$$T(7) = \frac{f(5) * T(5) + f(6) * T(6)}{f(7)} \qquad ....(9.16)$$

The synthesis gas then passes up through the catalyst bed cooler tubes where it is further preheated by heat exchange with the catalyst bed. The bed is divided into a number of increments as shown in Figure 9.4. Therefore, assuming the synthesis gas temperature is constant within each increment, the temperature of the symthesis gas leaving the ith increment is determined as follows :-

$$deltaTB(i) = \frac{Tc(i) - Tg(i-1) + Tc(i) - Tg(i)}{2} \qquad ....(9.17)$$

$$qbed(i) = UAbed * deltTB(i) \qquad ....(9.18)$$

$$Tg(i) = \frac{f(7) * Cpg * Tg(i-1) + qbed(i)}{f(7) * Cpg} \qquad ....(9.19)$$

where Tc(i) = ith catalyst bed incremental temperature

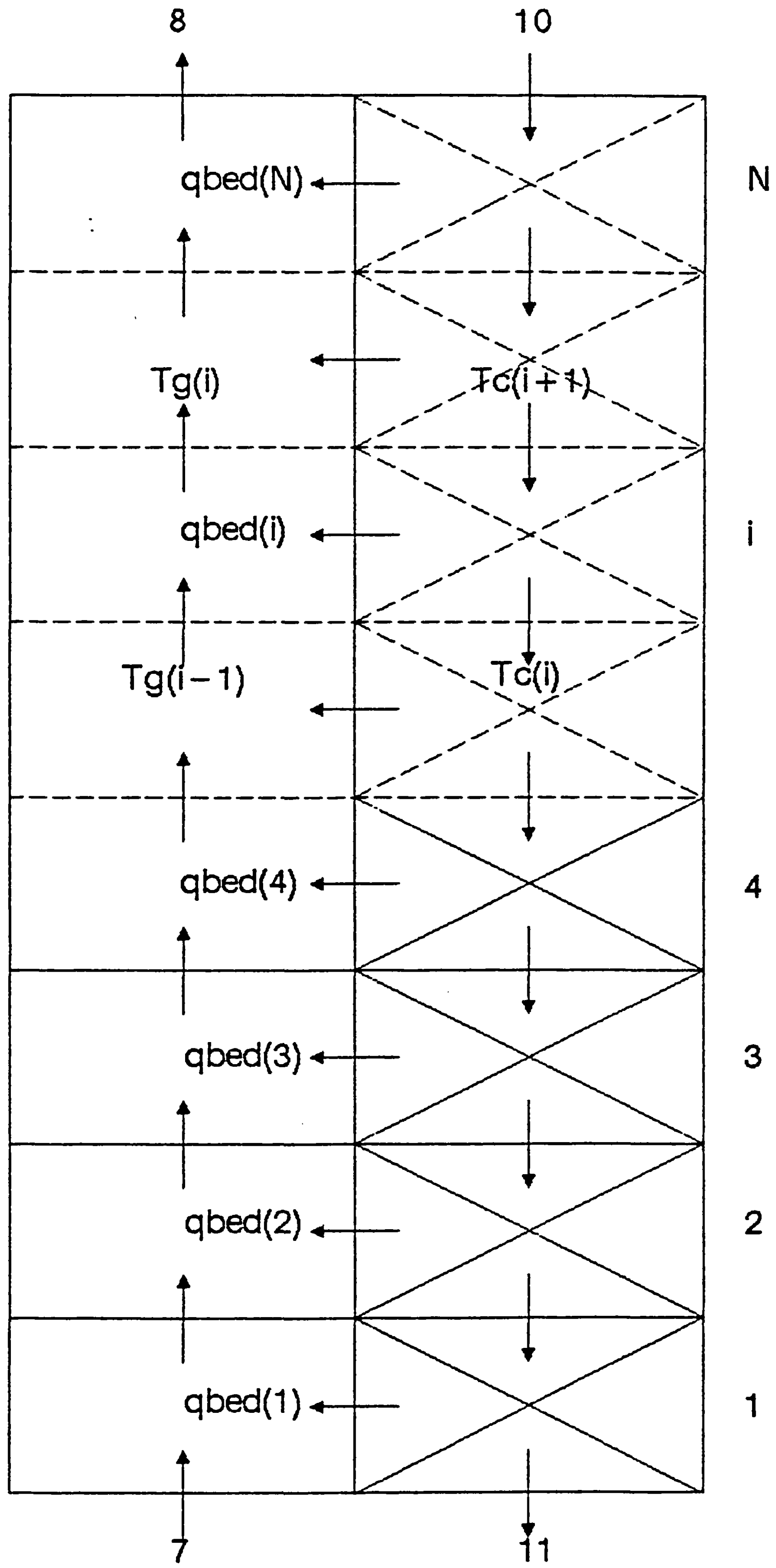
Tg(i) = synthesis gas temperature in ith catalyst bed cooler tube increment

deltaTB(i) = mean temperature difference between catalyst bed and synthesis gas in the cooler tubes in the ith increment

UAbed(i) = Overall heat transfer coefficient for ith increment

qbed(i) = Heat transfer rate between catalyst bed and synthesis gas in the cooler tubes in ith increment

Figure 9.4 : Ammonia Converter Catalyst Bed Model



The temperature of the synthesis gas exit the catalyst bed cooler tubes is then calculated :-

$$T(8) = Tg(N) \quad ....(9.20)$$

$$f(8) = f(7) \quad ....(9.21)$$

where N = no of catalyst bed increments

subscript 8 refers to synthesis gas conditions exit the catalyst bed cooler tubes

The direct bypass is then added back in to the synthesis gas flow as follows :-

$$f(10) = f(8) + f(9) \quad ....(9.22)$$

$$T(10) = \frac{f(8) * T(8) + f(9) * T(9)}{f(10)} \quad ....(9.23)$$

where subscript 10 refers to synthesis gas conditions exit addition of the direct bypass

The synthesis gas then passes down through the catalyst bed and ammonia is produced according to the reaction given in equation 9.1. The ammonia equilibrium and hence the amount of ammonia produced is modelled using a proprietary routine which is given in section 'ammrat' in lesson 'amconsim' in Appendix 3.10. This was converted directly from the fortran source code to the 'USE' language. The routine produces the change in the amount of amonnia for a given molar feed composition, synthesis gas pressure and catalyst bed reaction temperature.

The reaction temperature for the ith increment is calculated from the current value of temperature for that increment and the temperature of the preceeding increment which has just been calculated :-

$$Treact(i) = \frac{Tc(i) + Tc(i-1)}{2} \qquad ....(9.24)$$

where Treact(i) = reaction temperature

The synthesis gas pressure is updated via a simple expression which considers the molar flowrate of gas into and exit the shift converter as follows :-

$$Pc = Pc + (f(1) - f(15)) * C \qquad ....(9.25)$$

where Pc = synthesis loop pressure

C = constant

A value of the constant 'C' is chosen so that the change in synthesis loop pressure for a given change in the inlet molar flowrate, f(1) is comparable to the change that would be expected for the same change on the actual plant.

The routine 'ammrat' produces the change in number of moles of ammonia and therefore the component molar flows can be updated according to the stoichiometry given in equation 9.1 :-

$$y(i,1) = y(i+1,1) - 0.5 * dnh3(i) \qquad ....(9.26)$$

$$y(i,2) = y(i+1,2) - 1.5 * dnh3(i) \qquad ....(9.27)$$

$$y(i,3) = y(i+1,3) + dnh3(i) \qquad ....(9.28)$$

$$y(i,4) = y(i+1,4) \qquad ....(9.29)$$

$$y(i,5) = y(i+1,5) \qquad ....(9.30)$$

where $y(i,j)$ = jth component molar flow in the ith increment of the catalyst bed

$dnh3(i)$ = change in number of moles of ammonia in the ith increment of the catalyst bed

The component numbers can be found in Table 9.1.

The total molar flow of reacted gas in the ith increment of the catalyst bed, $fc(i)$ is then calculated as follows :-

$$fc(i) = y(i,1) + y(i,2) + y(i,3) + y(i,4) + y(i,5) \qquad ....(9.31)$$

This is then used to calculate the new catalyst bed temperature in the ith increment :-

$$Tc(i) = (fc(i+1)*Cpg*Tc(i+1) + Mc*Cpc*Tc(i) - qbed(i) + qreact(i))/(fc(i)*Cpg + Mc*Cpc) \qquad ....(9.32)$$

where Mc = incremental mass of catalyst in bed

Cpc = average catalyst specific heat coefficient

$qreact(i)$ = heat of reaction for ith increment

$$= dnh3(i) * Hreact \qquad ....(9.33)$$

$Hreact$ = heat of reaction per mole of ammonia

The temperature of the reacted gas exit the catalyst bed is then calculated :-

$$f(11) = fc(1) \qquad ....(9.34)$$

$$T(11) = Tc(1) \qquad ....(9.35)$$

where subscript 11 refers to the reacted gas condition exit the catalyst bed

If the boiler bypass molar flowrate is f(14) then the flow and temperature after the boiler bypass has been split are :-

$$f(12) = f(11) - f(14) \qquad ....(9.36)$$

$$T(12) = T(14) = T(11) \qquad ....(9.37)$$

where subscript 12 refers to reacted gas conditions exit the boiler bypass split

subscript 14 refers to the boiler bypass

The flow and temperature of the reacted gas exit the boiler is then calculated as follows :-

$$f(13) = f(12) \qquad ....(9.38)$$

$$T(13) = \frac{T(12) - Tb}{1.85} + Tb \qquad ....(9.39)$$

where Tb = temperature of saturated steam raised in boiler

subscript 13 refers to reacted gas conditions exit the boiler

Equation 9.39 is an empirical expression derived from plant experience. It was found that the amount of heat transfered in the boiler and hence the amount of steam raised was directly proportional to the flow of hot reacted gas through the boiler.

Finally, the boiler bypass is then added back to the reacted gas flow immediately after the boiler as follows :-

$$f(15) = f(13) + f(14) \qquad ....(9.40)$$

$$T(15) = \frac{f(13) * T(13) + f(14) * T(14)}{f(15)} \qquad ....(9.41)$$

These equations can then be solved using the algorithm shown in Figure 6.3 and described in section 6.4.3. The results of the calculations will be displayed on an animated mimic of the actual control room instrumentation. This enables the effects of the plant modifications to be demonstrated in a similar way to that on the plant. However, if the trainee makes a large change in one of the converter valve positions then a dramatic change in the steady state variables would result. In addition, the solution of the equations could become unstable. It is more important that the program exhibits a high degree of robustness rather than a high degree of accuracy. Therefore it is advantagous if the effect of any change in flowrate is broken down into smaller changes, each one a new steady state, so that the overall change proceed much slower.

The discharge coefficients of the four manual control valves are modelled using the routine 'valve' which is described in the 'simpac' manual in Appendix 2. The new steady state values for the synthesis gas feed, interchanger bypass and direct bypass flowrates are then calculated :-

$$ssf1 = cCv \qquad ....(9.42)$$

where $ssf1$ = synthesis gas feed steady state flowrate

cCv = circulation valve discharge coefficient

The interchange bypass steady state flowrate, ssf6 is calculated from equation 9.8 and the direct bypass steady state flowrate, ssf9 from equation 9.9.

The input flowrates for each loop of the steady state calculations are then calculated as follows :-

$$f(1) = f(1) + (ssf1 - f(1)) * C1 \qquad ....(9.43)$$

$$f(6) = f(6) + (ssf6 - f(6)) * C2 \qquad ....(9.44)$$

$$f(9) = f(9) + (ssf9 - f(9)) * C3 \qquad ....(9.45)$$

where C1, C2, C3 are constants

The values of C1, C2 and C3 were determined empirically so that the relative speeds of response of the three flowrates matched plant conditions. For example, a change in the circulation rate proceeeds much slower due to the amount of gas in the circulation loop than a change in say the interchanger bypass flowrate.

The 'USE' language code for the simulation calculations is given in section 'simcalcs' of lesson 'amconsim' which is given in Appendix 3.10.

9.2.3 The Program as Seen by the Trainee

A sample of the screen displays seen by the trainee are given in Figures 9.5 to 9.12. Figure 9.5 shows the opening display to the package and Figures 9.6 and 9.7 are examples of the screen displays used to describe the modifications to be made to the ammonia converter and their effects.

Figure 9.5 : Ammonia Converter Operation Title Screen

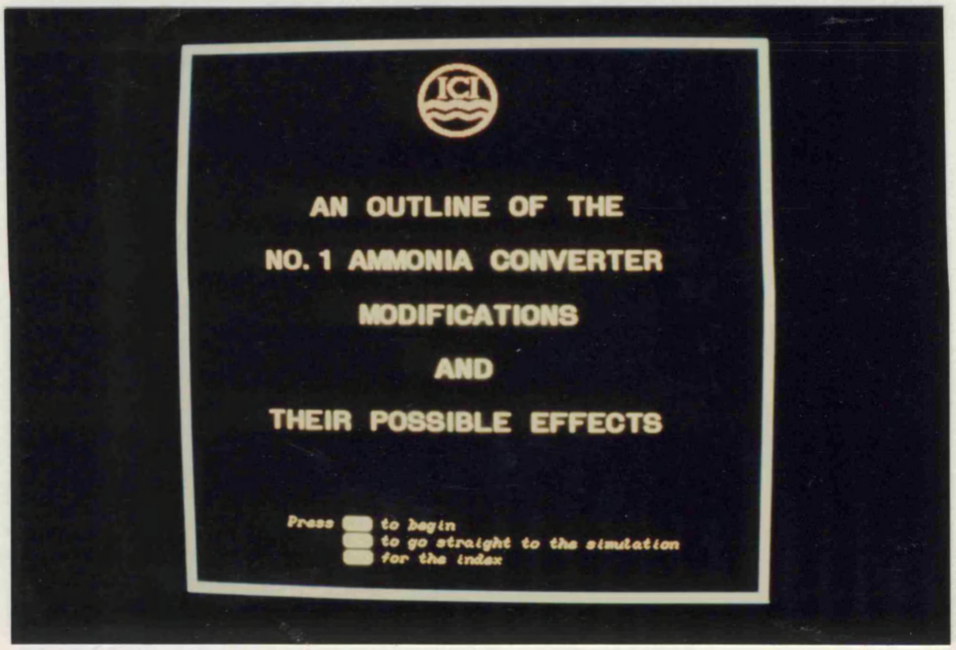


Figure 9.6 : Ammonia Converter Operation Introduction

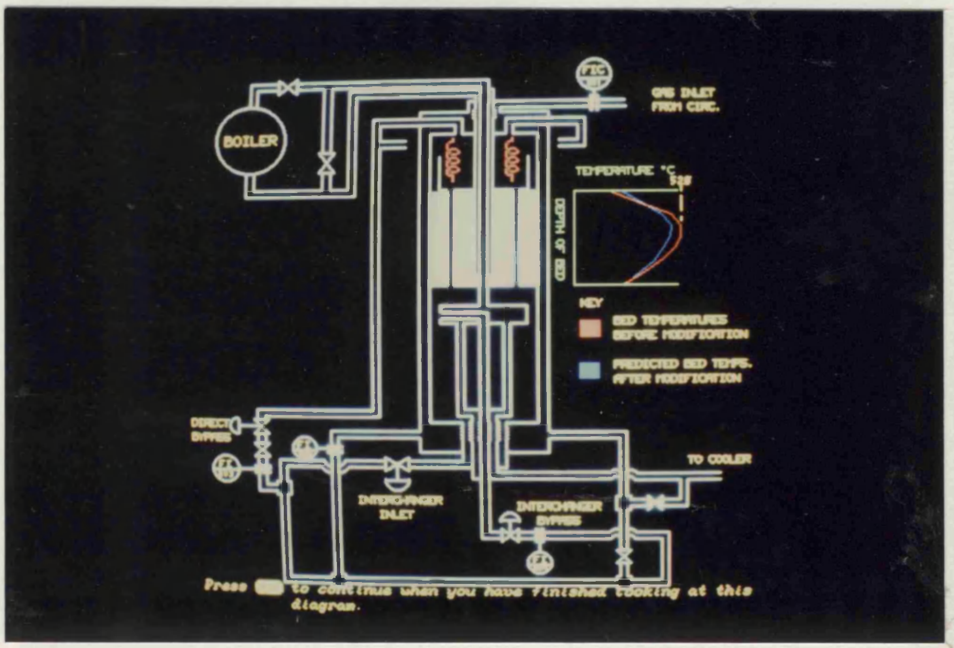


Figure 9.7 : Ammonia Converter Operation Introduction

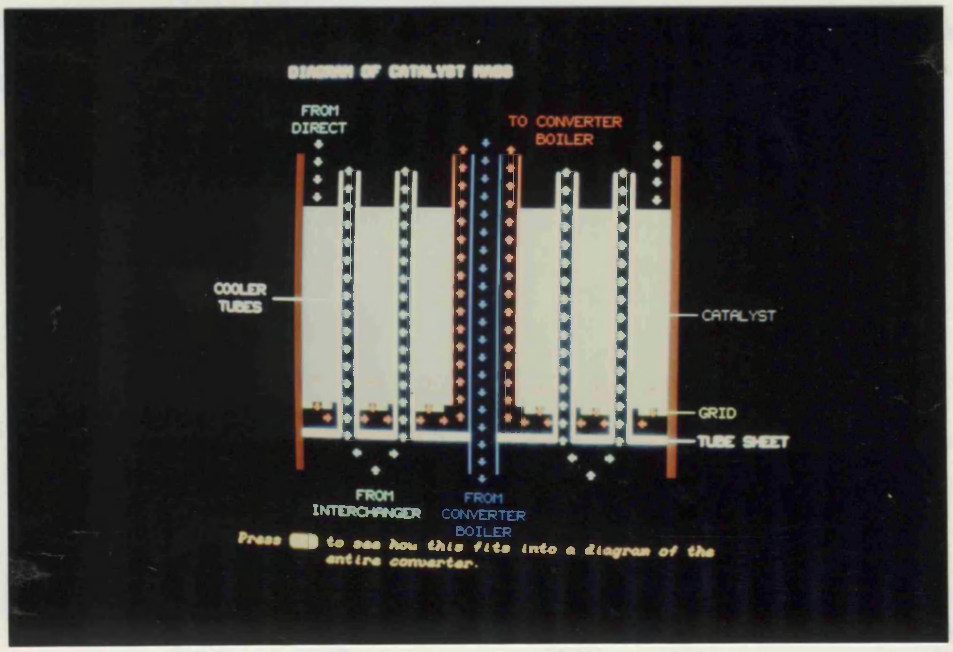


Figure 9.8 : Ammonia Converter Operation Simulation Title Screen

Figures 9.8 to 9.12 are samples of the screen displays from the third part of the package which allows the trainee to 'play' with the simulation. Figure 9.8 is the opening display.

Figure 9.9 shows the mimic plant control panel used to operate the simulation. Animated representations of the actual plant instrumentation are used. The relative positions of the individual instruments are retained on the condensed display. The mimic panel consists of three strip-chart recorders, one for the percentage ammonia in the synthesis gas fed to the converter, one for the converter catalyst bed temperatures and one for the make-up gas fed to the circulation loop.

The panel also features the four manually operated control valve displays for the circulation rate, direct bypass and interchanger inlet and bypass. The current values of the synthesis pressure, circulation rate, direct and interchanger bypass flowrates are shown on a number of analogue gauges. At the top of the panel there is a representation of part of the plant alarm panel. This includes all the alarms directly associated with the ammonia converter system. These will flash and annunciate in the normal way when particular values go out of bounds.

Figure 9.9 : Ammonia Converter Operation Mimic Plant Control Panel
Steady State Before Modifications

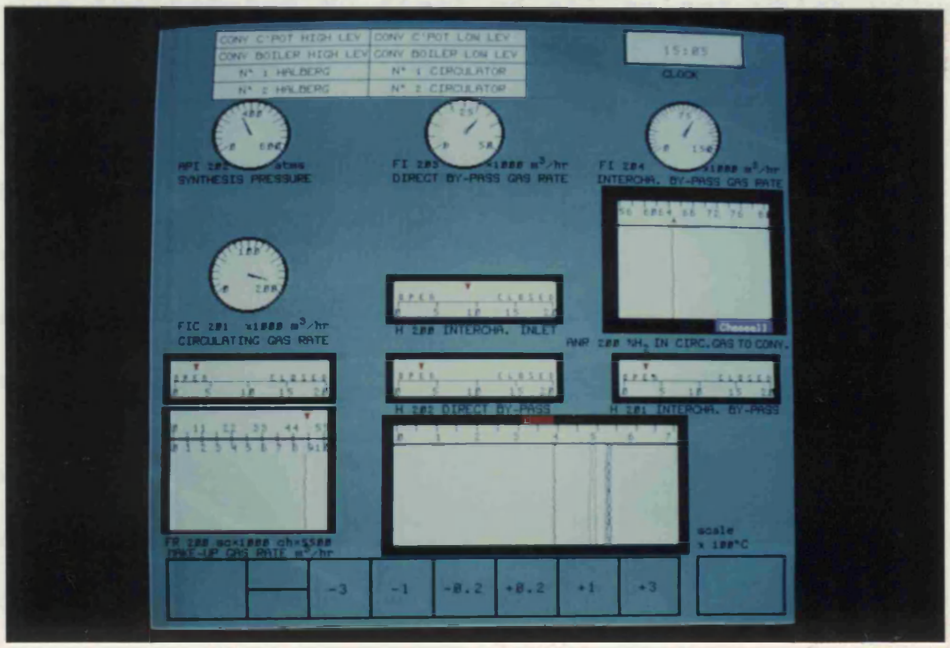
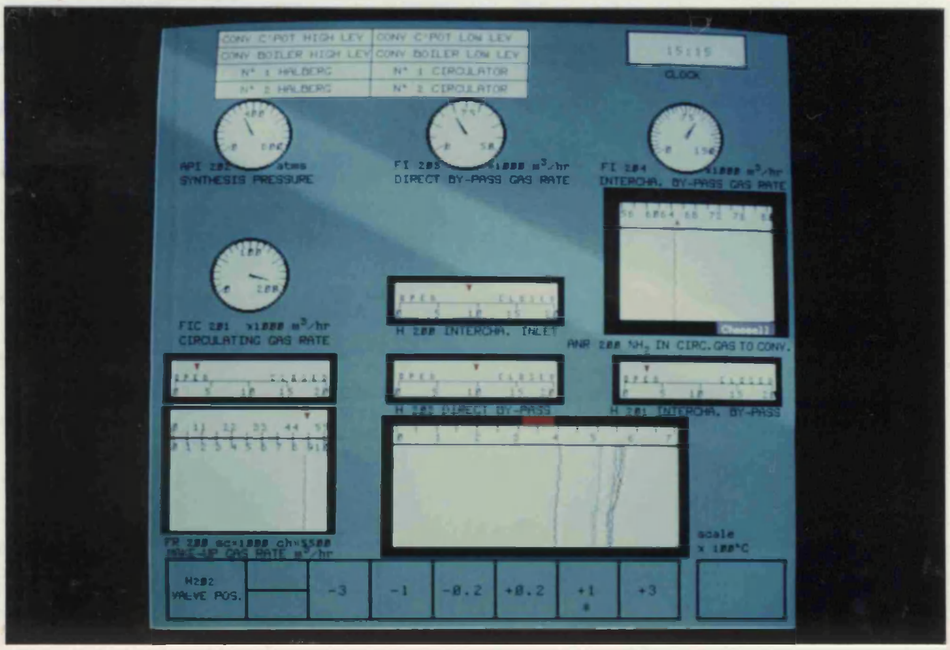


Figure 9.10 : Ammonia Converter Operation Mimic Plant Control Panel
Effect of Throttling Direct Bypass Before Modifications



A series of touch panel boxes is displayed at the bottom of the screen. In order to change the position of one of the valves, the trainee has to first of all select which valve he wishes to change by touching the appropriate valve display on the screen. Then, he can select the magnitude of the desired change by touching one of the option boxes which will be displayed for that particular valve. In this way the trainee can investigate the effect of a variety of different valve positions on the converter catalyst bed temperatures.

Figure 9.9 shows the system at steady state before the modifications have been made. Figure 9.10 shows the effect of throttling the direct bypass. Less cool synthesis gas is bypassed around the catalyst bed cooler tubes and therefore the temperature in the bed starts to rise as less heat is removed. This can cause significant damage to the catalyst if the temperature is allowed to rise too much.

Figure 9.11 shows the system at steady state after the modifications have been made. Comparing with Figure 9.9, it can be seen that the interchanger inlet flowrate has been increased by opening the inline valve and throttling the bypass. The direct bypass and the circulation rate have decreased slightly. The make-up gas rate has been increased to account for the extra ammonia produced. The catalyst bed temperatures have moved closer together. The lowest temperature has increased and the highest temperature has decreased.

Figure 9.11 : Ammonia Converter Operation Mimic Plant Control Panel
Steady State After Modifications

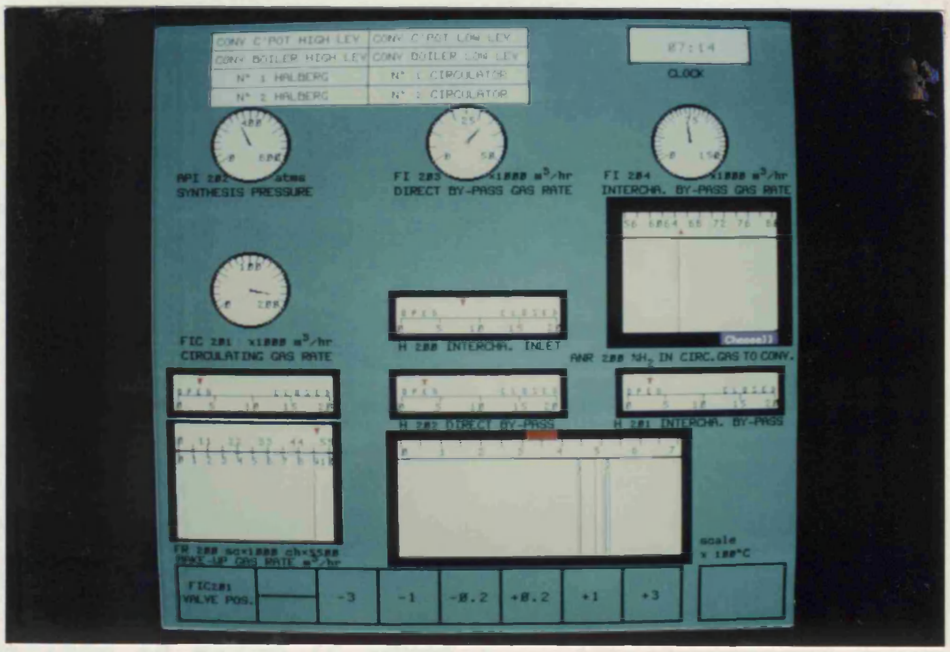


Figure 9.12 : Ammonia Converter Operation Mimic Plant Control Panel
Effect of Throttling Direct Bypass After Modifications

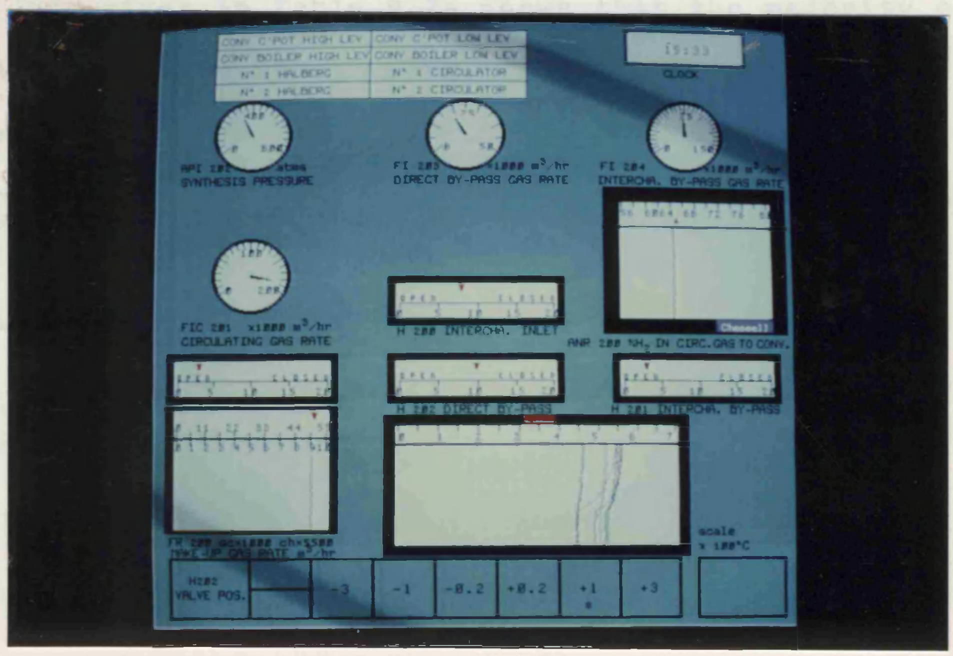


Figure 9.12 shows the effect of throttling the direct bypass still further after the modifications have been made. Notice that the catalyst bed temperatures have increased to a lower level than for the similar change before the modifications shown in Figure 9.10. However damage could still be done to the catalyst if care is not taken.

9.2.4 Comparison with Actual Plant Data

A comparison between the simulation and actual plant data before the modifications and predicted plant data after the modifications is given in Table 9.2. The percentage error is based on actual plant data where possible. The data covers most of the parameters which are displayed on the animated mimic control panel display.

Using the accuracy criteria set in section 6.5 of Chapter 6, the data given in Table 9.2a shows that the majority of the 'critical' parameters before the modifications are within 2-4% and therefore are fairly accurate. The exceptions to this are the interchanger inlet valve position and the inlet and exit catalyst bed temperatures. The error in the interchanger inlet valve position is 1 psig and the fidelity of the screen display does not really allow this error to be perceived.

Table 9.2 Ammonia Plant Ammonia Converter Operation
Plant/Simulation Comparison

Table 9.2a Before Modifications

	Plant	Design	Simulation	% Error
Critical Parameters				
Circ. Gas Flow(m3/hr)	178000	178000	178000	0
Synthesis Pressure(Bar)	320	320	320	0
Interchanger				
Bypass Rate(m3/hr)	41400	41400	41400	0
Inlet valve Position(psig)	8	-	9	12.5
Hydrogen in Circ. Gas(%)	-	64.3	64.3	0
Catalyst Bed Temperature Profile(C)				
Point 1	415	407	389	6.3
Point 2	445	453	432	2.9
Point 3	477	486	465	2.5
Point 4	505	509	490	3.0
Point 5	527	522	510	3.2
Point 6	532	522	524	1.5
Point 7	511	499	531	3.9
Point 8	436	445	462	6.0
Point 9	370	381	417	12.7
Non-critical Parameters				
Converter Exit Composition(%)				
Hydrogen	17	17.5	17.1	0.6
Nitrogen	52	52.5	51.2	1.5
Ammonia	21	21.4	23.0	9.5
Methane	4	4.4	4.4	10.0
Argon	4	4.2	4.3	7.5
Catalyst Bed Cooler Tubes Temperature Profile(C)				
Point 1	-	237	289	21.9
Point 2	-	314	343	9.2
Point 3	-	376	389	3.5
Point 4	-	424	428	0.9
Point 5	-	461	459	0.4
Point 6	-	486	484	0.4
Point 7	-	496	502	1.2
Point 8	-	487	509	4.5
Point 9	-	456	499	9.4

		Plant Design	Simulation	% Error

Table 9.2b After Modifications

Critical Parameters

		Plant Design	Simulation	% Error
Circ. Gas Flow(m3/hr)	-	175082	175083	0
Synthesis Pressure(Bar)	-	320	320	0
Interchanger				
Bypass Rate(m3/hr)	-	20000	20000	0
Inlet Valve Position(psig)	-	-	-	-
Hydrogen in Circ. Gas(%)	-	64.1	64.1	0
Catalyst Bed Temperature Profile(C)				
Point 1	-	410	444	8.3
Point 2	-	444	467	5.2
Point 3	-	471	486	3.2
Point 4	-	491	502	2.2
Point 5	-	505	514	1.8
Point 6	-	507	521	2.8
Point 7	-	492	518	5.3
Point 8	-	452	495	9.5
Point 9	-	400	448	12.0

Non-critical Parameters

		Plant Design	Simulation	% Error
Converter Exit Composition(%)				
Hydrogen	-	17.2	17.2	0
Nitrogen	-	51.7	51.5	0.4
Ammonia	-	22.3	22.6	1.3
Methane	-	4.5	4.4	2.2
Argon	-	4.4	4.3	2.3
Catalyst Bed Cooler Tubes Temperature Profile(C)				
Point 1	-	213	334	56.8
Point 2	-	271	370	36.5
Point 3	-	322	402	24.8
Point 4	-	365	430	17.8
Point 5	-	401	453	13.0
Point 6	-	430	472	9.8
Point 7	-	449	484	7.8
Point 8	-	455	487	7.0
Point 9	-	447	477	6.7

The inlet and exit catalyst bed temperatures seem to suffer from some end effects that have not been included which is not surprising since the modelling approach is fairly simple. The model could possibly be improved by increasing the number of increments used to model the catalyst bed as shown in Figure 9.4. However, this would increase overall calculation time and slow the response of the system to trainee changes. Alternatively, parameters such as the overall heat transfer coefficient for the end increments could be locally 'tuned' so that the simulated temperatures better reflect the plant/design values. However, the maximum and minimum temperatures within the simulated and the actual plant/design profiles do approximately agree. Since the operator only uses the range of temperatures to control the converter this inaccuracy is acceptable as long as the transient response shows the correct trends.

The 'non-critical' parameters given in Table 9.2a are all within the 10% criteria. The one exception to this is the catalyst bed cooler tube inlet temperature which also suffers from the previously mentioned end effect.

Examining the data in Table 9.2b, it can be seen that similar errors are obtained for the 'critical' parameters after the modifications. The accuracy of the 'non-critical parameters' varies widely. In particular, fairly large errors are obtained for the catalyst bed cooler tube temperature profile when compared to the design profile. These errors could possibly be reduced by including the heat capacity of the cooler tubes themselves. However, Table 9.2a shows that there is variation between the design and plant catalyst bed temperature profiles . Therefore it would be expected that there will also be variation in the catalyst bed cooler tube temperature profile. Since the converter exit composition agrees so well in Table 9.2b and the 'critical' catalyst bed temperature profile is sufficiently accurate then these errors can be tolerated.

It has been pointed out in section 6.5 of Chapter 6 that the best people to qualitatively evaluate the accuracy of the transient responses and the operational fidelity in general are the experienced senior control room operators and plant supervisors. Figure A4.17 in Appendix 4 shows that 8% of ICI Severnside's Ammonia Plant operators who responded to the questionnaire thought that the simulation response was good when compared to the actual plant. 69% thought the programs' response was 'ok' and just 23% thought that it was bad.

9.2.5 Discussion

This program was well received by plant personnel. Figure A4.12 in Appendix 4 shows that 55% of those who had seen the program considered it to be very useful and the remaining 45% considered it to be useful. Figure A4.18 in Appendix 4 shows that 8% of the Ammonia Plant Personnel who responded to the questionnaire considered that the Ammonia Converter Operation simulation had improved their knowledge of the plant a lot.

77% thought that the simulation had improved their plant knowledge a little and just 15% thought it had not improved their knowledge at all.

The recommissioning of the modified plant was successfully completed. Although the success of the startup cannot be directly related to the Ammonia Converter Operation simulation package, the Plant Manager believed that it had made a significant contribution.

This example demonstrates that a fairly simple modelling approach can be adopted for a complicated process and still achieve positive training results. It has already been pointed out in section 6.5 of Chapter 6 that the cost of developing the simulation rises slowly at first with increases in operational fidelity but then reaches a point where it rises much more steeply. This is a good example of where 80% of the benefits of the simulation can be obtained by modelling a small part of the entire system.

9.3 Ammonia Plant Reforming Section Operation

9.3.1 Introduction

This program simulates the 'cause and effect' operation of the reforming section of an ammonia plant. A schematic diagram of the process is given in Figure 9.13.

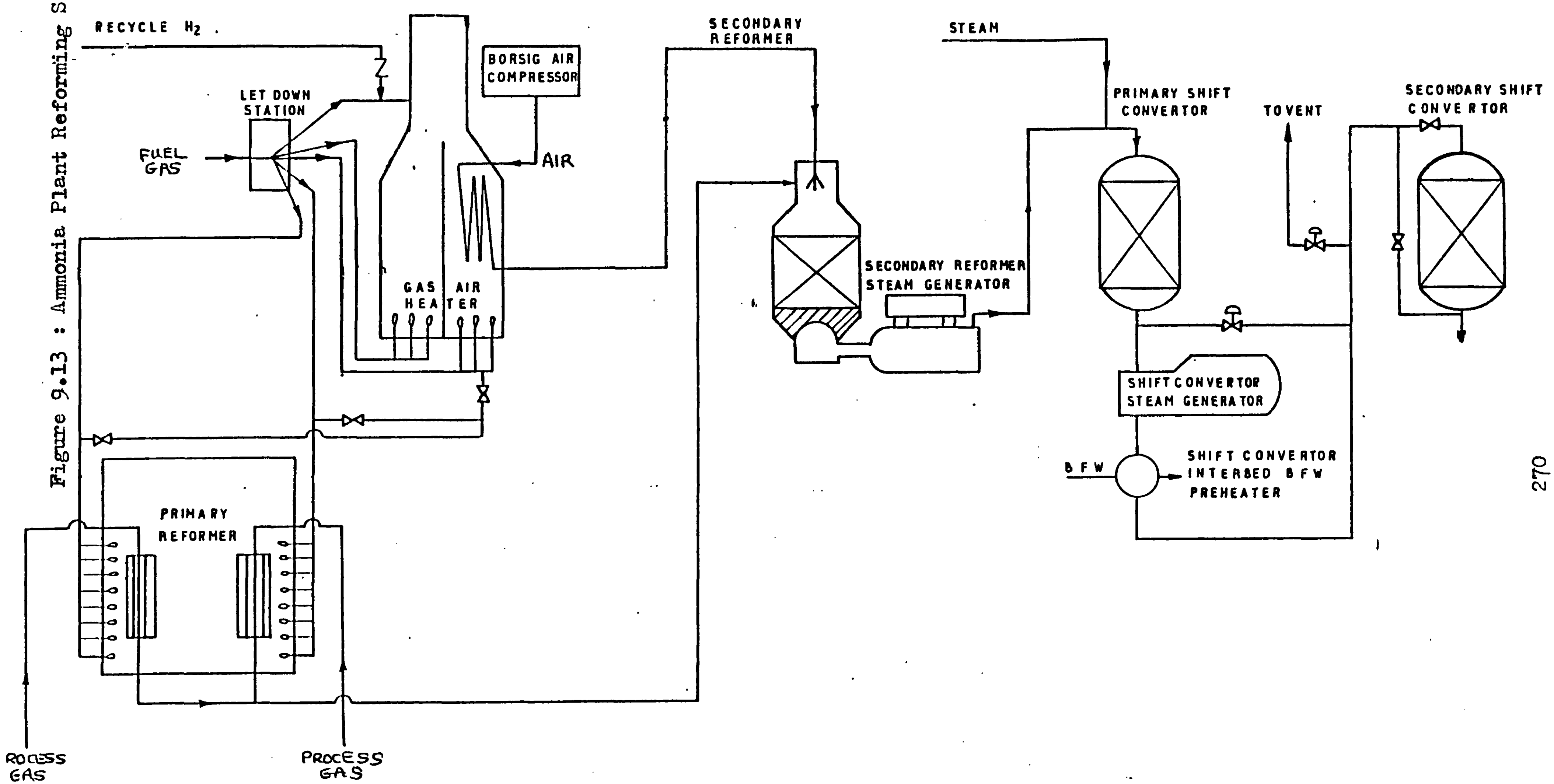


Figure 9.13 : Ammonia Plant Reforming Section

Methane in the form of natural gas plus steam and recycled hydrogen is fed to the primary reformer where it reacts according to two reactions as follows :-

$$CH_4 + H_2O \rightleftharpoons 3H_2 + CO \qquad \text{.......(9.46)}$$

$$CO + H_2O \rightleftharpoons H_2 + CO_2 \qquad \text{.......(9.47)}$$

The methane and steam produce further hydrogen plus carbon monoxide and carbon dioxide. The primary reformer is an externally fired tubular catalytic reactor. Natural gas is burnt in a box-type furnace through which the reactor tubes pass.

The gases from the primary reformer are then passed to the secondary reformer together with process air which has been preheated in the process gas air heater. The process gas air heater is a tubular furnace which is fired with natural gas. The secondary reformer is a catalytic bed reactor in which the remaining methane is reacted to produce further hydrogen.

The process gas exit the secondary reformer then passes through a boiler which cools the gas and raises steam. The process gas is then mixed with superheated steam and passed to the high temperature shift converter. The shift converter is a catalytic bed reactor which converts the carbon monoxide and steam to hydrogen by the water/gas shift reaction given in equation 9.47. The process gas then passes through a second boiler to generate further steam and then through the low temperature shift converter. The remaining carbon monoxide and steam react together to produce more hydrogen for the ammonia reaction which follows.

The program was developed to allow plant personnel to discover the 'cause and effect' relationships between the many process parameters associated with the Ammonia Plant reforming section. In normal circumstances, the plant operators are not able to carry out such investigations as the consequences of mis-operation are both dangerous and expensive. The simulation is operated from three animated mimics of the actual plant control room instrumentation. The trainee can change the main process parameters and observe the system's response on the animated display.

The objectives of the simulation are :-

(a) To demonstrate the 'cause and effect' relationship between the main process parameters associated with the Ammonia Plant reforming section.

(b) To demonstrate the steady state operation of the Ammonia Plant reforming section.

The structure of the program is as given in Figure 6.1. The 'USE' language code for the lessons '1as' and '1as1' which make up the reforming section operation program are given in Appendix 3.11. A brief description of the program as seen by the user is given in section 9.3.3. First of all, a description of the equations which model the operation of the system will be given in the next section 9.3.2.

9.3.2 Mathematical Model

The objectives of the program require that the 'cause and effect' relationships between the process parameters are modelled. Since the dynamics are not important then the 'steady-state snapshot' approach can be used. A proprietary material and energy balance for the Ammonia Plant reforming section was used to produce the simulation model. Only a brief description of the model equations can be given in this section.

Consider the system given in Figure 9.13. The mathematical model is divided into five sections as follows :-

- 9.3.2.1 Primary Reformer
- 9.3.2.2 Process Gas Air Heater
- 9.3.2.3 Secondary Reformer
- 9.3.2.4 High Temperature Shift Converter
- 9.3.2.5 Low Temperature Shift Converter

These will now be considered in turn.

9.3.2.1 Primary Reformer

The heat load and hence the reformer exit temperature is based on the firing rate in the furnace. However the exit temperature from the reformer is required to calculate the approach-to-equilibrium constants for the reaction and hence the exit gas composition. Therefore an iterative solution is required.

The firing rate, natural gas and steam feedrates and hydrogen recycle rates specified by the trainee are calculated as follows :-

firing = firing + (ssfiring-firing) * C1 ....(9.48)

natgasF = natgasF + (ssnatgasF-natgasF) * C2 ....(9.49)

pristeamF = pristeamF + (sspristeamF-pristeamF) * C3 ....(9.50)

hydF = hydF + (sshydF-hydF) * C4 ....(9.51)

where firing = primary reformer natural gas molar firing rate

ssfiring = trainee specified primary reformer natural gas molar firing rate

natgasF = primary reformer natural gas molar feedrate

ssnatgasF = trainee specified natural gas molar feedrate

pristeamF = primary reformer steam molar feedrate

sspristeamF = trainee specified primary steam molar flowrate

hydF = hydrogen molar recycle rate

sshydF = trainee specified hydrogen molar recycle rate

C1, C2, C3, C4 are constants

The constants C1, C2, C3, and C4 were determined empirically so that the relative speeds of response of the four flowrates matched plant conditions. The natural gas and steam feedrates and hydrogen recycle rate are used to calculate the primary reformer inlet composition, prin(i).

The reformer exit temperature, outpriT is then guessed. The routine 'reform' is used to calculate the exit gas composition from the reformer at this temperature based on reactions 9.46 and 9.47 :-

preff(i) = f(prin(i),outpriT,outpriP) ....(9.52)

where prin(i) = primary reformer inlet gas component molar flowrates

preff(i) = primary reformer exit gas component molar flowrates

outpriT = primary reformer exit temperature

outpriP = primary reformer exit pressure

A heat balance is then carried out as follows :-

Qpri = inpriH - outpriH + priHreact ....(9.53)

where Qpri = primary reformer heat load

inpriH = enthalpy of primary reformer inlet gas

outpriH = enthalpy of primary reformer exit gas

priHreact = primary reformer heat of reaction

The routine 'enth' is used to calculate the enthalpies of the inlet and exit streams using their composition, temperature and pressure.

The firing rate required to produce this heat load is then calculated from :-

cfiring = f(Qpri,outpriT) ....(9.54) where $cfiring$ = calculated primary reformer natural gas molar firing rate

The calculated firing rate, cfiring is then compared to that specified by the trainee, firing via the animated mimic control panel. The reformer exit temperature is updated and the calculations repeated until the two firing rates agree to within 1 %.

9.3.2.2 Process Gas Air Heater

The firing rate and secondary air flowrate specified by the trainee are calculated as follows :-

$$pahfire = pahfire + (sspahfire-pahfire) * C5 \quad \text{.......(9.55)}$$

$$secairF = secairF + (ssairF-secairF) * C6 \quad \text{.......(9.56)}$$

where $pahfire$ = process gas air heater natural gas molar firing rate

$sspahfire$ = trainee specified process gas air heater natural gas molar firing rate

$secairF$ = secondary air molar flowrate

$ssairF$ = trainee specified secondary air molar flowrate

C5, C6 are constants

The constants C5 and C6 are determined empirically as previously described.

A heat balance is then carried out to calculate the process air exit temperature :-

$$secairT = \frac{inairH + pahfire}{secairF * Cpa} \qquad ....(9.57)$$

where inairH = secondary air inlet enthalpy

inairT = secondary air inlet temperature

secairT = secondary air exit temperature

Cpa = specific heat capacity of air @ inairT

9.3.2.3 Secondary Reformer

The process gas from the primary reformer and the secondary air from the process gas air heater are mixed at the inlet to the secondary reformer. The routine 'enth' is used to calculate the enthalpy of the two streams from their composition, temperature and pressure. The process gas temperature is taken to be 20 degrees lower than the primary reformer exit temperature to account for heat losses. The routine 'tcalc' then calculates the mixed gas secondary inlet temperature.

An iterative solution, similar to that used for the primary reformer in section 9.3.2.1 is required to calculate the secondary outlet temperature and composition. The reformer exit temperature, outsecT and heat load, Qsec are guessed. The routine 'reform' is then used to calculate the exit gas composition from the reformer at this temperature based on reactions 9.46 and 9.47 :-

$$seceff(i) = f(\ secin(i), outsecT, outsecP\ ) \qquad ......(9.58)$$

where secin(i) = secondary reformer inlet gas component molar flowrates

seceff(i) = secondary reformer exit gas component molar flowrates

outsecT = secondary reformer exit temperature

outsecP = secondary reformer exit pressure

A heat balance is then carried out as follows :-

$$Qsec = insecH - outsecH + secHreact \quad ....(9.59)$$

where Qsec = secondary reformer heat load(Kcals)

insecH = enthalpy of secondary reformer inlet gas

outsecH = enthalpy of secondary reformer exit gas

secHreact = secondary reformer heat of reaction

The routine 'enth' is used to calculate the enthalpies of the inlet and exit streams using their composition, temperature and pressure. The calculations are repeated until two successive calculated heat loads agree to within 2 %. The guessed secondary reformer exit temperature is updated for each iteration based on the difference between the two heat loads.

9.3.2.4 High Temperature Shift Converter

First of all the boiler bypass valve position specified by the trainee is calculated as follows :-

$$bypass = bypass + (ssbypass-bypass) * C7 \quad ....(9.60)$$

where bypass = boiler bypass valve position

ssbypass = trainee specified bypass valve position

C7 is a constant

The constant C7 is determined empirically as previously described.

The bypass flow is then calculated using a manufacturers expression for the valve :-

$$bypassF = (0.4*bypass - 0.2*bypass*bypass) * outsecF \quad ....(9.61)$$

where bypassF = boiler bypass gas flowrate

outsecF = secondary reformer exit flowrate

The temperature exit the boiler is fixed since it is controlled at a specific value on the plant. The boiler heat load can then be calculated :-

$$Qboiler = A * (outsecF - bypassF)^{0.8} * deltaT \quad ....(9.62)$$

where Qboiler = boiler heat load

deltaT = boiler temperature difference

A is a constant

The constant A is determined empirically from plant experience.

The boiler heat load corresponds to the amount of heat removed from the process gas. Therefore the temperature exit the boiler once the bypass flow has been added back can then be calculated using the routine 'tcalc'.

Steam is then added to the process gas flow. The steam feedrate specified by the trainee is calculated as follows :-

$$secsteamF = secsteamF + (sssteamF-secsteamF) * C8 \quad ....(9.63)$$

where secsteamF = secondary reformer steam flow

sssteamF = trainee specified secondary steam flow

C8 is a constant

The constant C8 is determined empirically as previously described. The routine 'enth' is used to calculate the enthalpy of the process gas and steam from their temperature and pressure. The routine 'tcalc' is then used to calculate the inlet temperature to the high temperature shift converter, inhtsT.

An iterative solution, similar to that used for the primary reformer in section 9.3.2.1 is required to calculate the shift converter outlet temperature and composition. The high temperature shift converter exit temperature, outhtsT is guessed. The routine 'shift' is then used to calculate the exit gas composition from the shift converter at this temperature based on the water/gas shift reaction, equation 9.47 :-

$$htseff(i) = f(htsin(i),outhtsT,outhtsP) \quad ....(9.64)$$

where htsin(i) = high temperature shift converter inlet gas component molar flowrates

htseff(i) = high temperature shift converter exit gas component molar flowrates

outhtsT = high temperature shift converter exit temperature

outhtsP = high temperature shift converter exit pressure

A heat balance is then carried out as follows :-

$$Qhts = inhtsH - outhtsH + htsHreact \qquad ....(9.65)$$

where Qhts = high temperature shift converter heat load

inhtsH = enthalpy of high temperature shift converter inlet gas

outhtsH = enthalpy of high temperature shift converter exit gas

htsHreact = high temperature shift converter heat of reaction

The routine 'enth' is used to calculate the enthalpies of the inlet and exit streams using their composition, temperature and pressure. The heat load in the shift converter should be close to zero. The guessed shift converter exit temperature is updated for each iteration based on the calculated heat load until the heat load becomes zero.

9.3.2.5 Low Temperature Shift Converter

An iterative solution, similar to that used for the high temperature shift converter in the last section 9.3.2.4 is required to calculate the low temperature shift converter outlet temperature and composition. The shift converter exit temperature, outltsT is guessed. The routine 'shift' is then used to calculate the exit gas composition from the shift converter at this temperature based on the water/gas shift reaction 9.47 :-

ltseff(i) = f(ltsin(i),outltsT,outltsP) ....(9.66)

where ltsin(i) = low temperature shift converter inlet gas component molar flowrates

ltseff(i) = low temperature shift converter exit gas component molar flowrates

outltsT = low temperature shift converter exit temperature

outltsP = low temperature shift converter exit pressure

A heat balance is then carried out as follows :-

Qlts = inltsH - outltsH + ltsHreact ....(9.67) where Qlts = low temperature shift converter heat load

inltsH = enthalpy of low temperature shift converter inlet gas

outltsH = enthalpy of low temperature shift converter exit gas

ltsHreact = low temperature shift converter heat of reaction

The routine 'enth' is used to calculate the enthalpies of the inlet and exit streams using their composition, temperature and pressure. The heat load in the shift converter should be close to zero. The guessed shift converter exit temperature is updated for each iteration based on the calculated heat load until the heat load becomes zero.

These equations can be solved using the algorithm shown in Figure 6.3 and described in section 6.4.3. The results of the calculations will be displayed on three animated mimic displays of the control room instrumentation. This enables the 'cause and effect' relationships between the various process parameters to be observed in a similar way to that on the plant. However, if for example, the trainee makes a big change in one of the primary reformer inlet flowrates then a dramatic change in the steady state variables would result. As was discussed in section 6.4.3 it is advantageous for training purposes that any change in input parameters is broken down into smaller changes, each one a new steady-state, so that the overall change proceeds much slower.

This is achieved by the constants C1 to C8 which have been defined in the equations presented in this section.

The 'USE' language code for the simulation calculations is given in section 'simcalcs' and associated sections of lesson 'las' which is given in Appendix 3.11.

9.3.3 The Program as Seen by the Trainee

A sample of the screen displays seen by the trainee are given in Figures 9.14 to 9.17. Figure 9.14 shows the opening display to the package and the introduction which follows describes how to operate the simulation and some of the effects which can be studied.

When the trainee has been through the introduction he is then allowed to operate the simulation using the three animated control panels given in Figures 9.15 to 9.17. Figure 9.15 contains simple representations of the instruments associated with the primary reformer. It features two strip chart recorders for the temperature and methane composition exit the reformer and a series of touch panel boxes for changing the input flowrates such as the reformer fuel gas and the process steam.

Figure 9.14 : Ammonia Plant Reforming Section Operation Title Screen

Figure 9.15 : Ammonia Plant Reforming Section Operation
Mimic Primary Reformer Control Panel

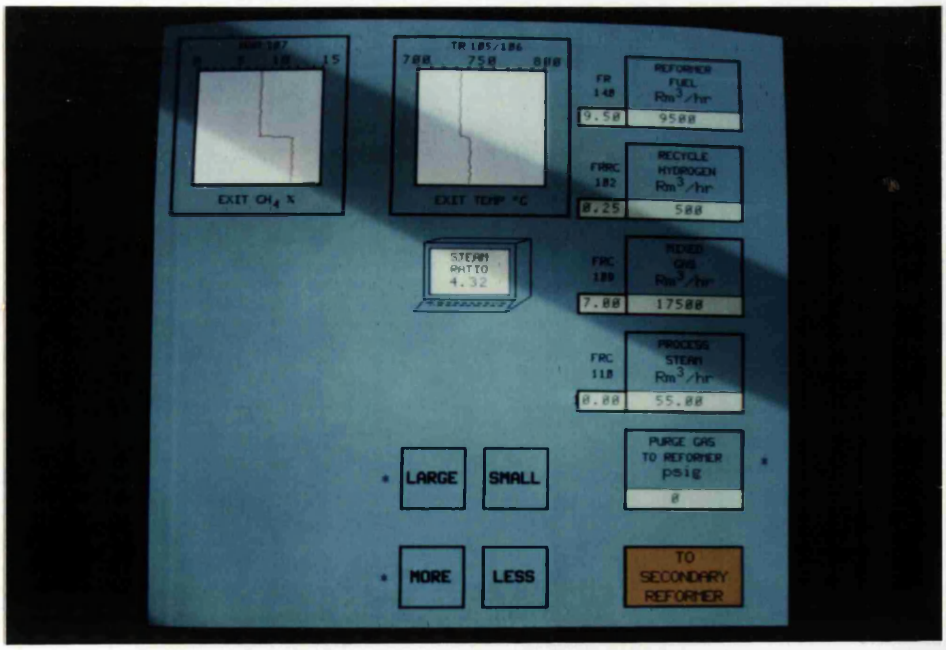


Figure 9.16 shows the instruments associated with the process gas air heater and the secondary reformer. There are also two strip chart recorders for the air temperature exit the process gas air heater and for the methane composition exit the secondary reformer. It also features a West Gardian temperature indicator for the secondary reformer exit temperature and touch panel boxes for changing the air flowrate and the secondary reformer fuel rate.

Figure 9.17 shows the instruments associated with the two shift converters. It features two strip chart recorder-controllers for the low temperature shift converter inlet temperature and the high temperature shift converter steam addition rate. In addition there are a multi-point temperature indicator and touch panel boxes for changing the setpoints of the two controllers.

Figure 9.15 to 9.17 shows the effect of an increase in the process steam fed to the primary reformer. More reaction occurs in both the primary and secondary reformers and therefore the methane composition exit each reformer decreases as shown in Figures 9.15 and 9.16. However, the increased reaction results in more carbon monoxide being produced. This is converted to hydrogen and carbon dioxide in the shift converters according to the water-gas shift reaction given in equation 9.47 . The increased reaction in the shift converters results in more heat being evolved and Figure 9.17 shows the warning that the temperature exit the high temperature shift converter is high.

Figure 9.16 : Ammonia Plant Reforming Section Operation
Mimic PGAH and Secondary Reformer Control Panel

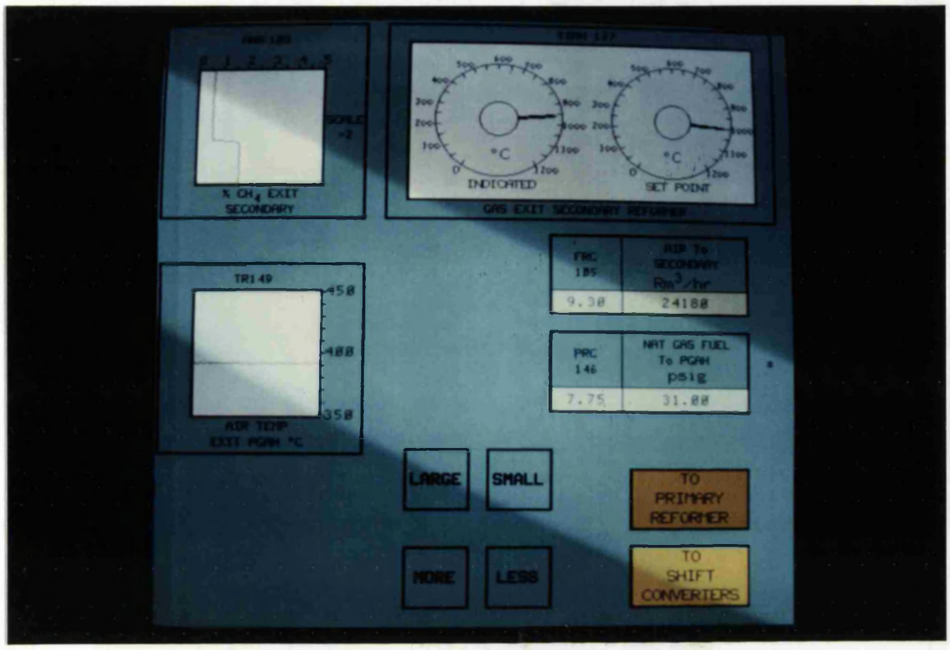
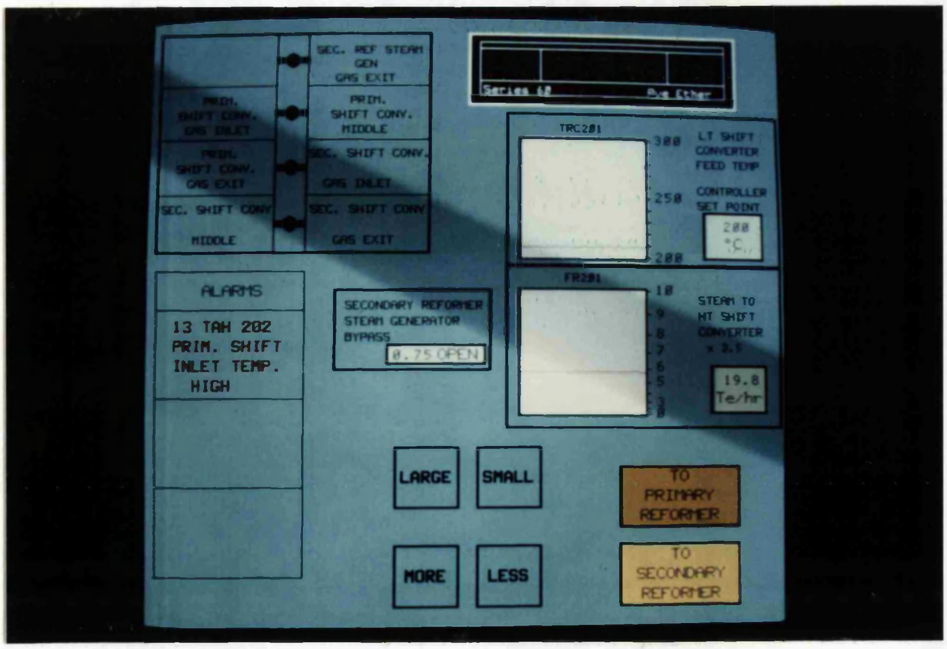


Figure 9.17 : Ammonia Plant Reforming Section Operation
Mimic Shift Converter Control Panel



9.3.4 Discussion

The program was also well received by plant personnel. Figure A4.13 in Appendix 4 shows that 31% of those who had seen the program considered it to be very useful, 56% considered it to be useful and just 13% considered it to be of no use. However, it is significant that those who considered it to be of no use were not from the Ammonia Plant area.

Chapter 10 Discussion

This study investigates the application of microcomputer-based simulation for training process plant personnel. Training simulations have been produced which enable a trainee to interact with a mathematical model of the plant's operation via an animated mimic of the actual plant's control panel instruments. These simulations have been well received by the plant personnel who have seen them and they have satisfied the training objectives for which they were written.

Process operating personnel require sufficient plant knowledge to monitor and operate the plant safely under normal conditions so that the required production is obtained at minimal cost. When abnormal conditions occur such as in the failure of plant equipment, the operators require operating skills such as fault detection and diagnosis so that the failure can be identified quickly and its effect on production minimised. The knowledge and skill required can only be obtained by experience and through training.

The combination of Computer-Based-Training and simulation coupled with the Open Learning approach enables a trainee to obtain dynamic, high quality training in the knowledge and skill of plant operation whenever it is needed. An operator with free time during a night shift can improve his plant knowledge and practise his fault diagnostic and decision making skills without having to wait for the availability of a training instructor or an expensive simulator.

If the microcomputer is installed adjacent to the plant control room then the operator can make direct comparisons between his training and the actual plant. This enables training to become part of his day-to-day job. Plant on-line time and overall efficiency can be maximised by the continual availability of a training and information resource.

I.C.I.'s Severnside Works have found that CBT is a more effective training method than conventional ones, with reduced training times being achieved. For example, using traditional training methods, it took fifteen weeks to train a new operator, but with CBT a new recruit has been accepted as being competent after only six weeks(I2).

The development of any microcomputer-based training simulation involves a number of stages. These stages are listed in Table 10.1. Once a process operating problem which requires training has been identified then the training programme should be developed following the guidelines given in section 3.3 of Chapter 3. A thorough analysis of the specific operator's task should be carried out to identify the actual knowledge and skill required by the operator to perform the task. The training objectives can then be specified, the training content determined and a suitable delivery media selected.

Table 10.1 Microcomputer-Based Training Simulation Development Steps

1.	Identify operating problem	
2.	Analyse operator's task	Section 3.3 Chapter 3
3.	Define training objectives and training content	Section 3.3 Chapter 3
4.	Select training delivery device	Section 3.5 Chapter 3 Section 3.6 Chapter 3
5.	Produce functional specification of simulation	Section 4.2 Chapter 4
6.	Identify process variables and and gather available plant data	Section 4.2 Chapter 4
7.	Select simulation equipment	Section 4.3 Chapter 4 Section 6.2 Chapter 6
8.	Develop simulation program	Section 6.3 Chapter 6
9.	Mathematical Modelling	Section 6.4 Chapter 6
10.	Design considerations	Section 6.5 Chapter 6
11.	Validate simulation	Section 6.5 Chapter 6
12.	Conduct training and obtain feedback	
13.	Modify and update as required	

A number of Open Learning delivery devices such as work books, slide/tape and video were described in section 3.5. In particular the use of Computer-Based-Training was described in section 3.6 of Chapter 3. The training objectives should determine which media is selected. For example, computer-based simulation should be used where the training objectives require that the trainee investigates the operation of a process in order to learn about the plant by discovery.

Plant training personnel should always be involved in identifying the training needs and defining the objectives. This ensures that a cost effective training simulation is produced rather than an elegant technical solution which tends to include irrelevant finer details. The current breed of microcomputers are not the vehicle for large scale detailed simulations of large sections of process plant and therefore clear, concise training objectives are neccesary for developing the simplified mathematical models which have to be used.

The development of training simulations was considered in section 4.2 of Chapter 4. First of all a functional specification for the simulation should be produced. This should identify the essential elements of the plant to be included in the simulation and usually results in a P & I diagram of the plant as it will be simulated. The next step is to identify the process variables to be included in the simulation and to gather any plant data which is available. The equipment on which the simulation is to be implemented can then be selected. The selection of microcomputer systems for interactive simulations was considered in section 6.2 of Chapter 6. A much higher degree of user interaction is required when using a microcomputer for training than is necessary when using the machine for other purposes. Good text and colour grahics are required to dynamically display the results of the simulation calculations on an animated mimic plant control panel. The trainee's keyboard skill cannot be assumed and so other means of interaction should be available such as a touch screen or a mouse.

The development and structure of the microcomputer-based training simulations presented in this work is described in section 6.3 of Chapter 6. The simulation programs are controlled by a main executive routine which calls all the other subroutines which make up the program. These subroutines include the instruction given to the trainee, the mathematical model of the process, the animation of the mimic plant control panels used to display the results of the simulation calculations and the control of how the trainee interacts with the system.

This study presents two alternative mathematical modelling approaches and these are described in section 6.4 of Chapter 6. The selection of which approach to use should be governed by the training objectives. For example, if the dynamics play an important part in the simulation such as in teaching the operation of process control systems, then a model which reproduces these dynamics should be used. If, on the other hand, the objective is to demonstrate the inter-relationships between process variables, then a model which represents these 'cause and effect' relationships should be used.

Dynamic simulation methods have been used to teach the operation and control of individual unit operations. The mathematical models used consist of simplified ordinary differential equations with model parameters such as overall heat transfer coefficients which are 'tuned' so that the model matches plant conditions to an acceptable degree of accuracy. The majority of the simulations also include fault diagnostic exercises. These are created by locally rewriting the model to simulate the process at that point, or by redefining input variables, so that abnormal operation is simulated and the changes proceed through the simulation.

The generic plant operation dynamic simulations presented in Chapter 7 and the specific plant operation dynamic simulations presented in Chapter 8 ably demonstrate the operation and control of individual unit operations. They enable the trainee to gain repeated and systematic practice in control loop operation and in fault diagnosis from control panel presented information which is an important area of understanding and one which is difficult to train 'on-the-job'. The generic plant operation simulations presented in Chapter 7 are particularly valuable in the initial training of control room operators because they demonstrate the principles of control without the distraction of a highly complex process.

'Cause and effect' simulation utilising steady-state material and energy balances has been used to give an overview of plant operations. For example, the simulation of Ammonia Plant Reforming Section Operation presented in section 9.2 of Chapter 9 demonstrates the effect of a change in steam input on the product produced. The Ammonia Converter Operation simulation presented in section 9.1 of Chapter 9 demonstrates how a fairly simple modelling approach can be adopted for a complicated process and still achieve positive training benefits. The cost of developing a simulation rises slowly at first with increases in operational fidelity but then reaches a point where it rises much more steeply. The

Ammonia Converter Operation simulation is a good example of where 80% of the benefits of the simulation can be obtained by modelling a small part of the entire system.

A highly accurate model is not required for training purposes, just one which reproduces the plant responses to a sufficient degree of fidelity so that the training objectives can be achieved. Differences between the simulation model and the actual plant's behaviour which do not materially affect the operator's judgement or do not result in an incorrect course of action will have a negligible effect in the training environment. It is more important that the program exhibits a high degree of robustness rather than a high degree of accuracy. However, caution should always be taken so that the trainee does not receive a too simplified view of the real world.

There is a limit in the scale of each type of simulation which can be effectively implemented on a microcomputer. The use of 'rate structuring' of the simulation calculations, screen animation and trainee interaction was discussed in section 6.5 of Chapter 6. There is a limit in both the scale of the mathematical model required to represent the system and the amount of screen animation required to mimic the plant control panel instrumentation at which a simulation of sufficient fidelity can be produced. This limit is reflected in not being able to operate the simulation in real-time or faster. In this case a more powerful machine such as a workstation is required.

Once the training simulation program has been completed it should be validated against the available plant data. The accuracy criteria used in this study are defined in section 6.5 of Chapter 6. The simulations should also be extensively validated by a number of experienced senior control room operators and supervisors. They will know the plant responses better than anyone else and will be only too willing to tell you where the simulation is inadequate. The use of the simulation outside of the range of existing plant data and experience should be treated with extreme caution. In particular, if a potential hazardous situation could arise then the simulation should be suspended and the trainee given a severe warning on the consequences of his actions. The author, in conjunction with plant management, should ensure that the validation is carried out thoroughly since he will be responsible in the event of the simulation misleading the trainees into an incorrect course of action which could have dire consequences.

The final stage in the development of the training simulation package is to carry out the training with a number of actual trainees for a sufficient period to generate enough information on the effectiveness of the material. The package should then be modified or updated based on the feedback obtained to improve its efficiency of achieving the training objectives.

The time taken to develop Computer-Based-Training material varies with the complexity of the material. Author preparation/trainee hour ratios of 75:1 for tutorial-mode CBT and 200:1 for simulation-mode CBT have been reported(B2).

However, these ratios depend on the definition of one hour of training time. The development time of simulations presented in this work can be classified according to whether the simulations are generic or plant specific. The generic simulations can be developed in a few weeks and development times of 4-8 weeks are typical for those presented here. The plant specific simulations which involve extensive validation require a much longer time and development times of the order of months are typical. These times could obviously vary substantially depending on the complexity of the simulation and the expertise of the author.

The development time and cost of microcomputer-based training simulation when compared to full scale replica plant control room simulators is significantly less. For example, a full scale simulation for Ammonia Converter Operation would have cost at least ten times more to develop. This study has demonstrated that small scale, relatively low cost solutions can be developed to satisfy process plant personnel training needs.

The potential benefits of microcomputer-based training are numerous and varied. The obvious advantage is that new and existing process operators can be trained in the intricacies of plant operation without risking loss of life or injury to other personnel and/or loss of production due to equipment downtime. Plant efficiences can be improved by training the operators to control the plant within tighter limits. It enables the quantitative effects of minor changes in process conditions on efficiency and product yield to be demonstrated. Plant safety can be improved since the operator can practice his diagnostic skills and therefore help him to recognise earlier the propagation of faults which could lead to hazardous situations.

Microcomputer-based simulator training enables the learning environment to be controlled. The control may be over the degree of complexity of the task the trainee encounters. For example, the trainee could be given a simple task or parts of the overall task or a general outline of the system before being given the full complexity of the task. Better feedback can be given on the trainee's actions than would occur if the trainee was being trained on-the-job. It enables precise instructional objectives to be set with appropriate remedial action for trainees who fail to reach the required level.

It is very difficult to quantify the value of microcomputer-based process plant personnel training. The benefits are reflected in increased output and reduced downtown over a long period of time. Its value can also be demonstrated through increased knowledge, skill, motivation and confidence on the part of process plant personnel. The opinions of plant personnel were obtained from a questionnaire the results of which are presented in Appendix 4. Figure A4.14 shows that, in general, 31% of those who had seen any of the simulations thought that they had improved their plant knowledge a lot and the remaining 69% thought that they had improved their knowledge a little.

However, it is significant to note that less than half of the questionaires issued were returned and approximately one third of the people who did return questionaires had not seen any of the simulations. The full commitment of plant management is required from an early stage in the development of microcomputer-based training. This should ensure that the full co-operation of plant personnel is given in developing, and more importantly, in validating the training simulations. The degree of success in achieving the benefits of microcomputer-based training is dependent on support from plant management in encouraging plant personnel to use the resources available and in giving feedback on a trainee's post training performance to reinforce the correct operational practices.

The production of microcomputer-based training simulations could be aided by the development of a library of simulation routines such as the one called 'simpac' started in this work. This library should be similar to those already available to the engineer for the design and analysis of process plant but should include the facilites to simulate abnormal plant behaviour such as the sticking of control valves and the leaking of vessels.

Microcomputer-based simulation training could be further enhanced in the future by the application of recent developments in both computer hardware and software. Cheaper computer hardware will bring computer-based-training within the reach of a wider variety of companies. Increasing power of microcomputers will allow larger scale training simulations to be implemented and more detailed mathematical models to be used.

Interactive video will allow the trainee to observe and interact with a video picture of the actual plant control panel with which he will be working. Computer animation can be overlayed on top of the video picture to mimic the movement of the various gauges and indicators. The trainee can also be shown a video sequence on how to find plant valves which have to be opened manually. Digital audio could be used to record the noise associated with a process plant. These noises such as a compressor stopping or a particular alarm signal could be played back via the computer at the appropriate point in the simulation. In this way training simulations of much greater fidelity could be created on a microcomputer.

The application of expert system technology could be used to further enhance the learning experience. The expert system could be used to monitor trainee actions and to advise on the operating procedures to be followed by the trainee where necessary. In addition, it could give guidance on fault diagnostic procedures and direct the trainee to remedial instruction when a lack of understanding is identified. The combination of an expert system and microcomputer-based training simulation is currently being investigated(K7),(M17).

Appendix 1 Microcomputer Hardware And Software For Interactive Simulation

1.1 Regency Computer-Based-Training System

The Regency microcomputer system was developed specifically for computer-based-training applications(T5). It is the third generation of a system whose development was started in 1965 by Paul Tenczar at the University of Illinois. Tenczar created five basic commands, 'unit', 'at', 'write', 'arrow' and 'answer'. These made the writing of instructional programs much less cumbersome and much more interactive than was possible with high level scientific languages such as 'FORTRAN'(T3).

The 'TUTOR' authoring language, as it became known, was used as the basis of the PLATO(Programmed Logic for Automated Teaching Operations) CBT system. This consisted of a mainframe computer, trainee delivery stations and the equipment necessary to interact with these stations(T6). PLATO is now a trademark of the Control Data Corporation and has found wide use in both education and industry(E2),(S2),(T1).

In 1977, the 'TUTOR' authoring language was transformed into the 'USE' authoring language by Urbana Software Enterprises for implementation on the Regency microcomputer manufactured by Regency Systems Inc. of Champaign, Illinois(T5). The highly specialised R-1 microcomputer-based-training system was launched in 1979. Regency and the 'USE' language, like its predecessor, PLATO and the 'TUTOR' language, has continually evolved since then into probably the most comprehensive CBT authoring system available today. The current R-2C hardware will be described in the next section 1.1.1 and the 'USE' authoring language will be discussed in section 1.1.2.

1.1.1 Regency Hardware

The Regency R2-C microcomputer system is available in several configurations. It consists of a system unit with display, keyset and either a twin floppy disk drive unit or a drive unit containing a hard disk drive and a floppy disk drive. In addition, a second display screen can be added. A typical configuration is shown in Figure A1.1.

Figure A1.1 : The Regency R2-C Microcomputer System

The 14in display units each contain a 512 x 512 array of individually addressable dots. The high resolution makes it possible to create complex graphics, easy-to-read text or to integrate both in a single display. The R2-C has a total display area of 1024 x 1024 dots. The display area can be divided into four seperate 512 x 512 displays or accessed in the full 1024 x 1024 mode. In the four screen mode the author can choose to plot into a non-displayed screen area while waiting for a trainee keypress. After the trainee has pressed a key, the author can switch instantly to display the prepared screen area. The ability to plot on one screen area while another is displayed eliminates any apparent display plotting time. In the full 1024 x 1024 mode the author can display a large, complex panel from which the trainee can select those functions required for a given lesson segment by moving the 512 x 512 displayed 'window' of the display area. The R2-C also has the capability to zoom in on a particular section of the display. This allows the user to get a more detailed look at any part of the display.

The main display unit also includes a touch panel which allows the user to interact directly with the computer by touching the screen. Realistic simulations can be executed without using the keyset. The touch panel operates in one of three modes, point, stream or continuous. In point mode, only one point is detected each time that the screen is touched. In stream mode, points are detected as the user moves a finger across the screen but single touches are not detected.

The basic system unit memory configuration consists of 64 Kbytes of main or central memory(RAM). In addition, there is 256 Kbytes of auxiliary mass storage(AMS), which serves as a temporary buffer for data or programs that cannot or need not reside in central memory. The buffer storage serves to decrease the apparent access time of the disk drives or to reduce the number of communications over a network. An additional 512 Kbyte bit-mapped memory is dedicated to the screen display. The R2-C can produce 256 different shades of colour and display up to 16 of these colours on the screen at any one time. The author specifies which of the 256 shades to use by selecting a 'palette'(R7).

The Regency R2-C can be used stand alone or networked to a central hard disk drive unit. This enables a trainee station to be placed on each plant so enabling a training and information resource to be available 24 hours per day, 7 days per week. The Regency network at ICI's Severnide Works is shown in Figure A1.2.

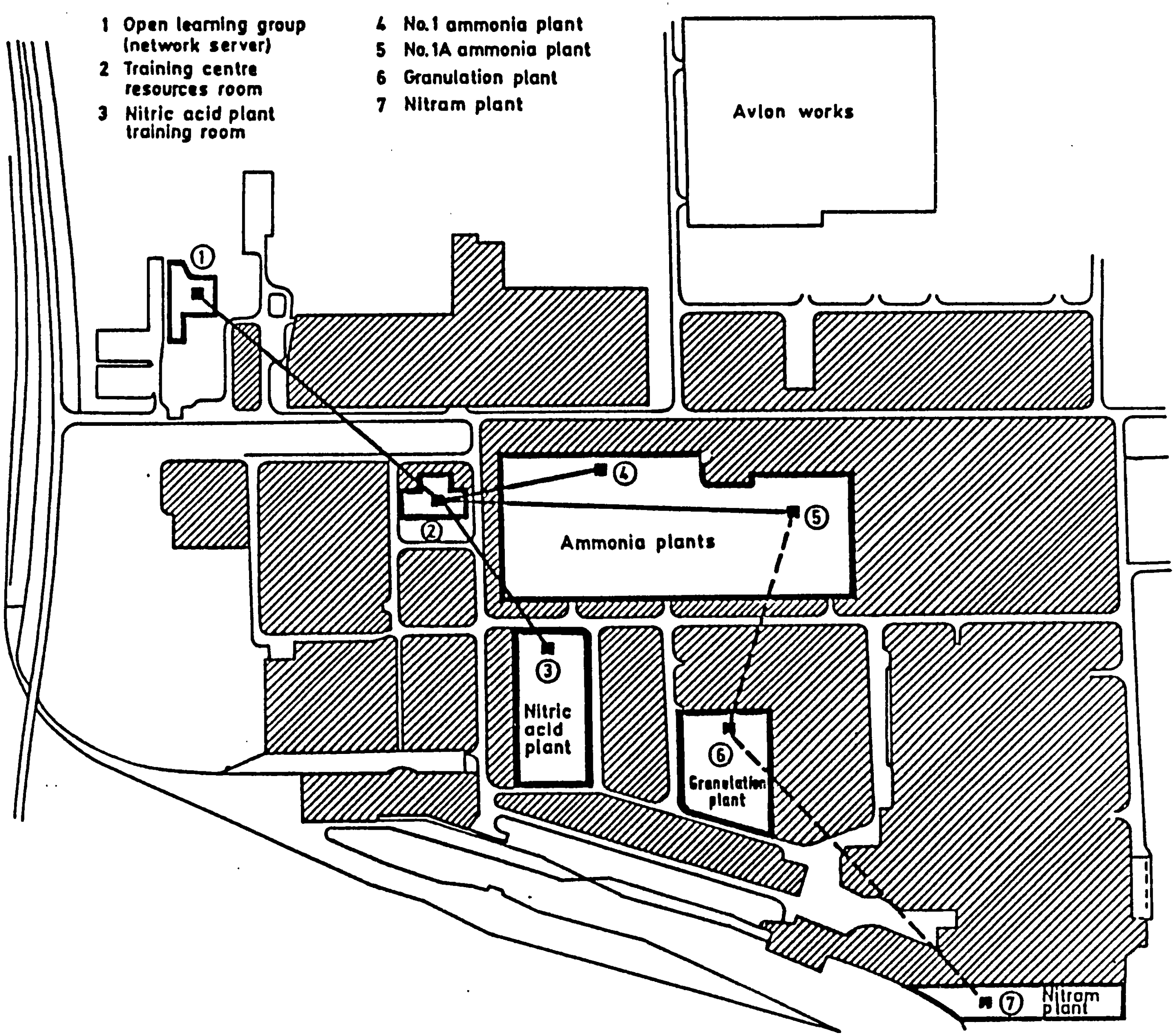


Figure A1.2 : ICI's Severnside Works Regency Microcomputer Network

1.1.2 Regency R2-C Operating System

The Regency Operating System allows three types of users to access the system. These users may be :-

(a) Trainees

(b) Instructors

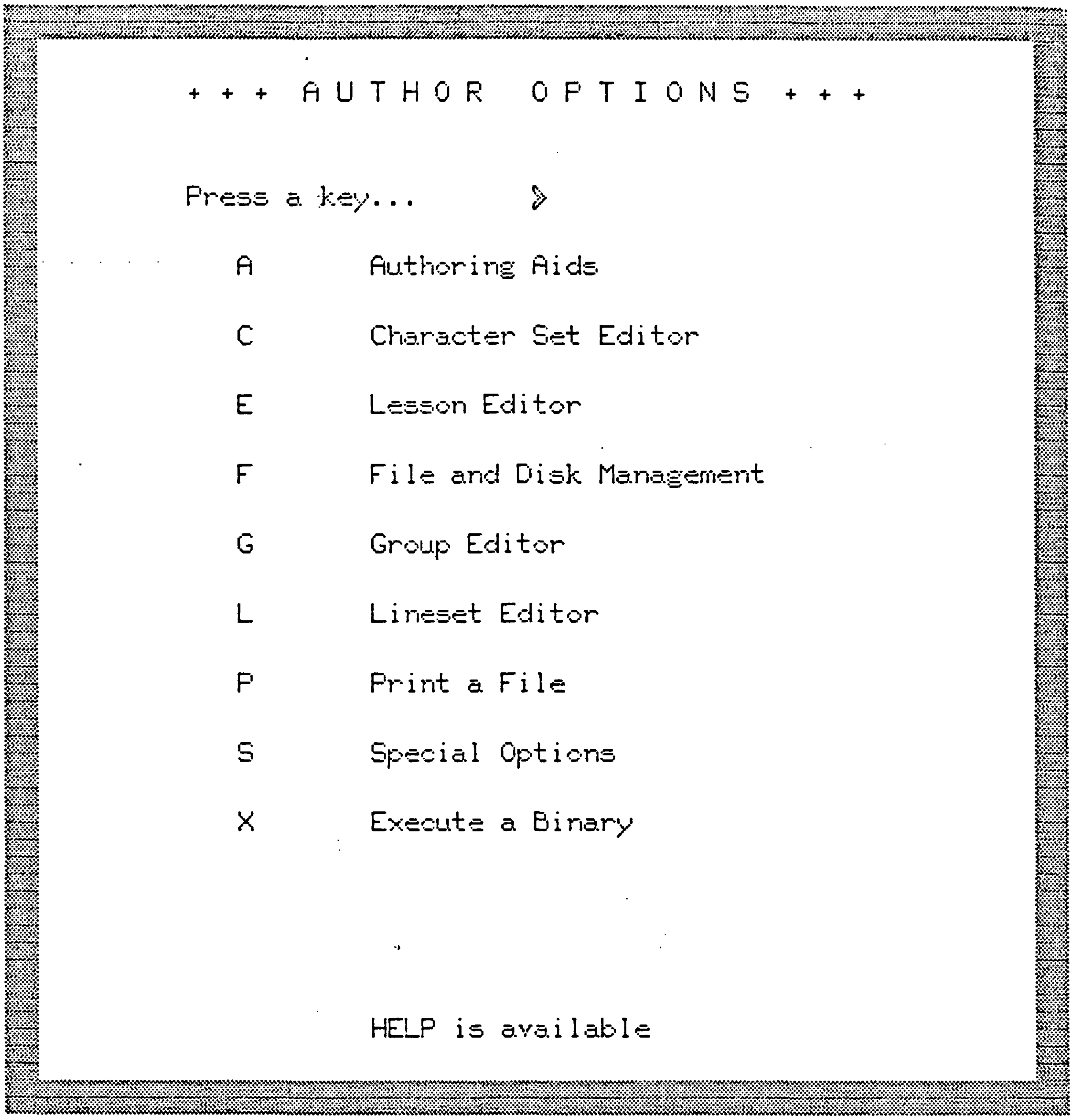
(c) Authors.

Trainees can only execute the programs specified by the author or his instructor. Instructors can execute all programs and examine trainee records which are created by the management system. Authors can execute any of the programs available and also create and edit lessons.

The Regency authoring system is menu-driven. Figure A1.3 shows the main 'Author Options' menu(R7). 'Authoring Aids' is a complete on-line reference manual describing the tools of lesson programming such as 'USE' language define structures, system reserved words, and the function and syntax of each 'USE' command.

The 'Character Set Editor' enables the author to create and change dot-matrix patterns on an 8 x 16 matrix, each one being associated with a keypress. You can also design and edit these characters on a multiple display showing a 64 x 64 dot-matrix to enable large characters made up of a number of keypresses to be created.

Figure A1.3 : The Regency Operating System Menu Screen



The 'Lesson editor' enables the author to write source code for lessons. You can add, delete, reorder and edit sections of lessons and lesson source code. A display editor enables you to create and change screen displays as they are viewed and automatically inserts the corresponding source code into the the lesson. An 'Aids-on-page' facility lets you see a description of 'USE' commands while you are editing. The 'USE' language will be described in the next section 1.1.3.

'File And Disk Management' allows the author to allocate and control space on a disk. The 'Group Editor' option allows the author to manage access to the system via the use of sign-on rosters. The 'Print a file' option allows lesson source code to be printed out and 'Execute a lesson' enables any condensed(compiled) lesson to be executed.

The 'Lineset Editor' is similar to the 'Character Set Editor' but the composition of the characters or drawings consists of lines rather that dots. Line-drawn characters are both sizeable and rotatable where as dot characters are not.

'Special Options' includes features which are rarely used such as options to inspect and edit files byte-by-byte, to initialise the unit buffer, to select the primary disk drive and to run hardware tests.

1.1.3 The 'USE' Language

The 'USE' language provides an English-like set of commands especially adapted to the needs of interactive programs and instructional lessons. It has an efficient block structure, good implicit branching, powerful answer-judging capabilities for both numerical and character data and it lends itself to efficient structured programming. It provides an organisational framework on which an efficient instructional dialogue can be constructed.

Therefore, training simulations can be written to interpret user responses, branch appropriately based on such responses and perform specialised repetitive operations that are essential for user-machine interaction. Mathematical models can be created easily and efficiently since the computational capability of 'USE' is comparable to most advanced scientific languages such as 'FORTRAN77'.

Authors find the English-like commands easy to remember and use. For example, in one day's work, a typical author could write 2 to 5 times as many instructional units in 'USE' as he could in a language primarily intended for computation such as BASIC or FORTRAN and 10 or more times as much as he could in assembly language(R8).

A comparison is given in Table A1.1 between 'USE', BASIC and FORTRAN to demonstrate the significant features of the 'USE' language.

Table A1.1
Comparison of the 'BASIC', 'FORTRAN' and 'USE' Languages

	'BASIC'	'FORTRAN'	'USE'
Arithmetic Expressions			
	*	*	x or *
	/	/	÷ or /
	+	+	+
	-	-	-
	^	**	**
Logical Operators			
	<=	.LE.	≤
	<	.LT.	<
	>	.GT.	>
	>=	.GE.	≥
	=	.EQ.	=
	<>	.NE.	≠
Logical Expressions			
	10 IF x>= y THEN S1	if x.GT.y go to S1	if x≥y . branch S1 endif
	10 IF E < 0 THEN S1 20 IF E = 0 THEN S2 30 IF E > 0 THEN S3	if E.LT.0 S1 if E.EQ.0 S2 if E.GT.0 S3	if E<0 . branch S1 elseif E = 0 . branch S2 elseif E >0 . branch S3 endif
		if x=y S1,S2	branch x=y,S1,S2,S3
Remark/Comment Statements			
	10 REM______________	C____________	*__________ $$__________ can be used on the same lines as a command statement
Variable Names			
	eg. A A1	Name Variable up to 6 characters eg. APPLE1	Name Variable up to 8 characters eg. Apple123
Integer Variables			
		I,J,K,L,M,N are taken as integers. This can be avoided by declaring these as real eg. REAL K.	Defined as integers in defines section of program eg. i,2 The 2 refers to the size of the storage location, in this case 2 bytes long.

Table A1.1 continued.

	'BASIC'	'FORTRAN'	'USE'
Input/Output of Data			
	10 LET x = 10 20 LET y = 100	x = 10 y = 100	Calc x ⇐ 10 y ⇐ 100
	10 INPUT x	read (,),x Device Label 5 for input Format Statement Label	screen co-ordinate arrow → 2080 judge OK store x endarrow
	10 DATA 1.0 20 READ x	data x/1.0 read (5,10),x	
	10 PRINT x	write (,),x Device Label 6 for output Format Statement Label	screen co-ordinate at → 1020 write x,2,1 digits before dec.pt digits after dec.pt
DO-Loops			
	10 FOR I = 1 TO N . . . . 100 NEXT I	do 100 I=1,N specifies last statement of loop	loop I ⇐ 1,N . . . . endloop
Nested DO-Loops		do 10 I=1,N read (5,100),T(I) do 20 J=1,M 20 read (5,200),T(I+N) 10 continue	loop I ⇐ 1,N . store T (I) . loop I ⇐ 1,M . . store T (I+N) . endloop endloop
Subroutines			
	GOSUB 600 ← line number of start of subroutine	call intde (x,dx) subroutine name	do intde(x,dx) arguments

1.2 Other Microcomputer Systems

1.2.1 Interactive Simulation On Microcomputers Using 'BASIC'

There are some attempts reported using microcomputers and the 'BASIC' language for producing interactive simulations. Haynes(H5) used a BBC model B microcomputer with 32K RAM to simulate the operation of a forward-feed double effect evaporator. The simplified dynamic simulation model was written in 'BBC BASIC'. The results of the simulation calculations were displayed on simple monochrome graphic displays. The displays were produced using a package called 'DESIGN' from Beebugsoft(P3). This enabled the displays to be stored on disk and loaded into screen memory as required. This ensured that the maximum amount of the 32K RAM was available for the 'BBC BASIC' simulation program. User interaction was achieved via keypresses and a menu displayed at the bottom of each screen display.

Ellison and Tunnicliffe Wilson(E3) describe a similar program written in 'Applesoft BASIC' for the Apple II microcomputer which simulates four batch reactors in parallel. McDermott(M14) has also produced an interactive simulation of an evaporator control system using a low level 'BASIC' on the Sinclair QL and BBC model B microcomputers. Once again simple monochrome graphic displays were used and user interaction was achieved via keypresses.

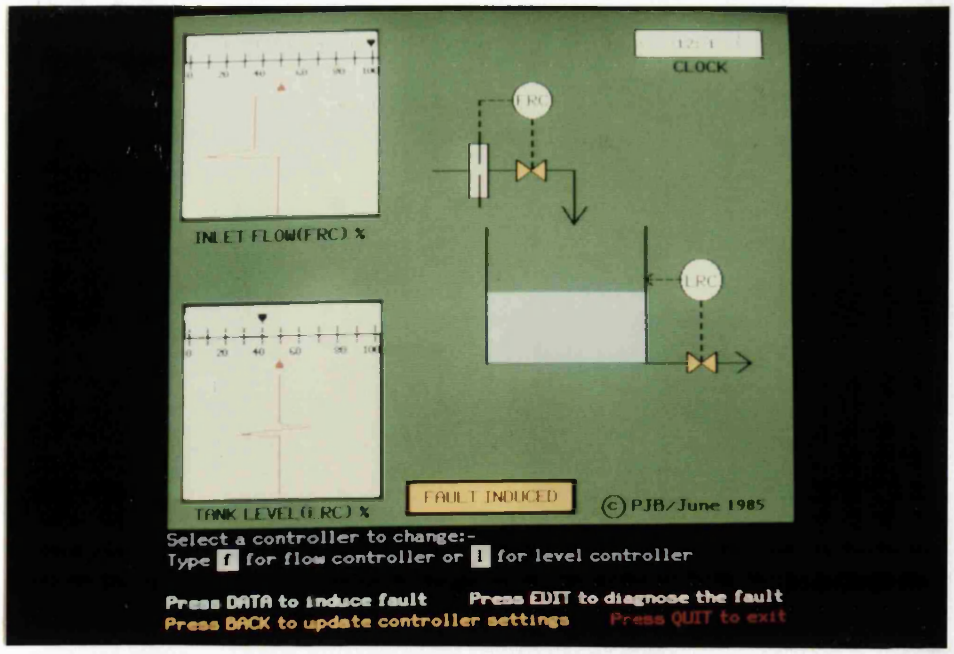
The three programs described all suffer from poor graphical display facilities and from limited user interaction. The 'BASIC' language enables only simple interaction via keypresses to be programmed and does not allow an instructional dialogue to be created with the trainee. It is also difficult to produce detailed graphic displays without resorting to other packages and then the quality which can be produced is limited by the microcomputer hardware employed.

1.2.2 Interactive Simulation On IBM PC XT Using TenCORE

The IBM PC XT microcomputer offers an attractive environment on which to produce interactive simulations. It can utilise a variety of graphics cards to produce a number of colour graphic displays from low to high resolution. User interaction can be achieved via the keyboard or a mouse. Floating-point calculations required for the simulation model can be executed quickly using an 8087 maths co-processor and up to a maximum of 640K RAM of memory can be installed in the machine.

A simulation of a simple tank level control system similar to the one described in section 7.3 was implemented on an IBM PC XT of the above configuration with a Tecmar colour graphics card and using the TenCORE Authoring Language(B3). TenCORE is a fourth generation language which has been produced by Tenczar to follow on from the highly successful 'TUTOR' and 'USE' languages. It is essentially just an IBM PC implementation of its predecessors with additional features to utilise the various hardware configurations of the IBM PC. The Tecmar card produces sixteen colour graphics on a 512 x 480 or 640 x 400 dot resolution display. Animated colour graphics were used to display the results of the simulation calculations on a mimic plant control panel as shown in Figure A1.4 to produce a real time representation of the process. Facilities are included to introduce various faults and disturbances into the simulation. Answer judging routines were constructed to compare the trainee's diagnosis of these faults with the correct answer with feedback being given where necessary. Criteria for mastery can be set and the trainee's progress through the simulation controlled until the required level is reached.

Figure A1.4 : Tank Level Control Simulation Using TenCORE



1.2.3 Interactive Simulation Using MicroTICCIT

MicroTICCIT is a computer-based-instructional system which has been used extensively in training both operators and maintenance personnel in the USA(W3). It can simulate actual equipment with computer-generated graphics or video materials or both simultaneously. Wilson and Kilgore(W3) describe its use in pilot and maintenance training. In particular it has been used to produce dynamic simulations of aircraft fuel systems where fuel use at varying speeds and under normal and failed conditions is demonstrated.

MicroTICCIT runs on a local area network of IBM PC's or compatibles with a Data General microECLIPSE minicomputer as a host unit. The screen display is limited to 11 colours at any one time. User interaction is achieved via a keyboard or a touch screen. Computer-generated graphics can be overlayed onto video pictures to create highly realistic training presentations. However, the initial capital cost of the system is high due to the necessity of the Data General host unit.

Appendix 2

'simpac'
A 'USE' Language Simulation Routine Package

2.1 Copy of 'simpac' user manual

Appendix 3 'USE' Program Listings

3.1 Steam-Heated Heat Exchanger Control

3.2 Tank Level Control

3.3 Co-Current Heat Exchanger Control

3.4 Counter-Current Heat Exchanger Control

3.5 Manual By-Pass Heat Exchanger Control

3.6 Continuous Stirred Tank Reactor Control

3.7 Continuous Binary Distillation Control

3.8 Nitric Acid Plant Ammonia Vaporiser Control

3.9 Ammonia Plant Make-Gas Boilers Control

3.10 Ammonia Plant Ammonia Converter Control

3.11 Ammonia Plant Reforming Section

Appendix 4 Simulation Evaluation

4.1 Introduction

In order to obtain a qualitative evaluation of the interactive simulation a questionnaire was prepared to obtain the opinions and views of plant personnel of I.C.I.'s Severnside Works who had had the opportunity to use the programs. Three questionnaires were prepared and these are given in the next section 4.2. Each questionnaire contains a number of general questions about the simulations together with more specific questions about the simulations relevant to a particular plant. The questionnaires were distributed to three groups of process operators and to instrument/electrical technicians as shown in Table A4.1 below.

The data obtained from the questionnaires is given in graphical form in section 4.3 together with other relevent comments expressed on the questionnaires.

Table A4.1 Number of Questionaires Issued

Granulation	30
Instrument/Electrical	58
Nitric Acid	19
No 1 Ammonia	21
TOTAL	128

4.2 Questionnaires

4.2.1 Granulation Plant And Instrument/Electrical Questionnaire

<u>Simulation's Questionnaire</u>

Please answer all questions by ticking the appropriate boxes.

1. Have you seen any of the simulation programs on the Regency computer ?

YES	NO

If your answer is NO to the above question please just return the questionnaire without answering any further questions.

2. How useful do YOU think that the following general simulations are ?

	Haven't Seen It	NOT Useful	Useful	VERY Useful
(a) Tank Level Control				
(b) Co-Current Heat Exchanger				
(c) Counter-Current Heat Exchanger				
(d) Steam-Heated Heat Exchanger				
(e) Stirred Tank Reactor				
(f) Manual By-pass Heat Exchanger				

3. How useful do YOU think that the following plant simulations are ?

	Haven't Seen It	NOT Useful	Useful	VERY Useful
(a) Nitric Acid Plant Ammonia Vaporiser Control				
(b) No1 Ammonia Plant Ammonia Converter				
(c) No1A Ammonia Plant Reforming Section				

4. Do you feel that your knowledge of process plant operations has been improved by using the above simulation programs ?

NONE	A LITTLE	A LOT

5. Which of the following do YOU think simulations are useful for ? Please tick all you think apply and add any of your own suggestions to the list.

(a)	Demostrating faults	
(b)	Demonstrating changes in plant operating conditions due to modifications	
(c)	Giving you the opportunity to 'play' with the plant	
(d)	Improving your knowledge of the plant's responses	
(e)	Improving your knowledge of the plant's operation	
(f)	.... (please add)	

6. Please add any further comments you may have in the space below. eg, are there any simulations you would like to see available ? Are there any parts of your plant you would like simulated ?

Please return your completed questionnaire to:

Peter Billing
Open Learning Group
HQ Block

Thank you for you help.

4.2.2 Nitric Acid Plant Questionnaire

<u>Simulation's Questionnaire</u>

Please answer all questions by ticking the appropriate boxes.

1. Have you seen any of the simulation programs on the Regency computer ?

YES	NO

If your answer is NO to the above question please just return the questionnaire without answering any further questions.

2. How useful do YOU think that the following general simulations are ?

	Haven't Seen It	NOT Useful	Useful	VERY Useful
(a) Tank Level Control				
(b) Co-Current Heat Exchanger				
(c) Counter-Current Heat Exchanger				
(d) Steam-Heated Heat Exchanger				
(e) Stirred Tank Reactor				
(f) Manual By-pass Heat Exchanger				

3. How useful do YOU think that the following plant simulations are ?

	Haven't Seen It	NOT Useful	Useful	VERY Useful
(a) Nitric Acid Plant Ammonia Vaporiser Control				
(b) No1 Ammonia Plant Ammonia Converter				
(c) No1A Ammonia Plant Reforming Section				

4. Do you feel that your knowledge of process plant operations has been improved by using the above simulation programs ?

NONE	A LITTLE	A LOT

5. How well does the response of the Nitric Acid Plant Ammonia Vaporiser simulation compare to the response of the actual plant to similar changes ?

BAD	OK	GOOD

6. Do you feel that your knowledge of the Nitric Acid Plant has been improved by using the Ammonia Vaporiser simulation ?

NONE	A LITTLE	A LOT

7. Which of the following do YOU think simulations are useful for ? Please tick all you think apply and add any of your own suggestions to the list.

(a) Demostrating faults	
(b) Demonstrating changes in plant operating conditions due to modifications	
(c) Giving you the opportunity to 'play' with the plant	
(d) Improving your knowledge of the plant's responses	
(e) Improving your knowledge of the plant's operation	
(f) .... (please add)	

8. Please add any further comments you may have in the space below. eg, are there any simulations you would like to see available ? Are there any parts of your plant you would like simulated ?

Please return your completed questionnaire to:

Peter Billing
Open Learning Group
HQ Block

Thank you for you help.

4.2.3 No 1 Ammonia Plant Questionnaire

Simulation's Questionnaire

Please answer all questions by ticking the appropriate boxes.

1. Have you seen any of the simulation programs on the Regency computer ?

YES	NO

If your answer is NO to the above question please just return the questionnaire without answering any further questions.

2. How useful do YOU think that the following general simulations are ?

	Haven't Seen It	NOT Useful	Useful	VERY Useful
(a) Tank Level Control				
(b) Co-Current Heat Exchanger				
(c) Counter-Current Heat Exchanger				
(d) Steam-Heated Heat Exchanger				
(e) Stirred Tank Reactor				
(f) Manual By-pass Heat Exchanger				

3. How useful do YOU think that the following plant simulations are ?

	Haven't Seen It	NOT Useful	Useful	VERY Useful
(a) Nitric Acid Plant Ammonia Vaporiser Control				
(b) No1 Ammonia Plant Ammonia Converter				
(c) No1A Ammonia Plant Reforming Section				

4. Do you feel that your knowledge of process plant operations has been improved by using the above simulation programs ?

NONE	A LITTLE	A LOT

5. How well does the response of the No 1 Ammonia Plant Ammonia Converter simulation compare to the response of the actual plant to similar changes ?

BAD	OK	GOOD

6. Do you feel that your knowledge of the No 1 Ammonia Plant has been improved by using the Ammonia Converter simulation ?

NONE	A LITTLE	A LOT

7. Which of the following do YOU think simulations are useful for ? Please tick all you think apply and add any of your own suggestions to the list.

(a) Demostrating faults	
(b) Demonstrating changes in plant operating conditions due to modifications	
(c) Giving you the opportunity to 'play' with the plant	
(d) Improving your knowledge of the plant's responses	
(e) Improving your knowledge of the plant's operation	
(f) .... (please add)	

8. Please add any further comments you may have in the space below. eg, are there any simulations you would like to see available ? Are there any parts of your plant you would like simulated ?

Please return your completed questionnaire to:

Peter Billing
Open Learning Group
HQ Block

Thank you for you help.

4.3 Questionnaire Results

The following figures are presented which summarise the responses obtained from the questionnaires :-

The questionnaire also gave the opportunity for each individual to make comments regarding interactive simulations. It was suggested that further programs should be developed to demonstrate :-

- Nitric Acid Plant Start-Up Procedures
- Nitric Acid Plant Rate Changes
- Nitric Acid Plant Overview

In addition it was felt that a simulation should be at the centre of any training package which involved plant control and operation. It was stated that simulations were very useful in training new personnel and for refresher training. They had helped tremendously in allowing self-teaching of other plants. However, it was felt that Plant Supervisors should give encouragement to learn about the operation of other plants.

The Instrument/Electrical section thought that some of the faults demonstrated in the programs were too simple and repetitive. They also would like greater access to the Regency System by having a network terminal available in Redwick Works Engineering Block.

Fig A4.1: Granulation

Questionaires

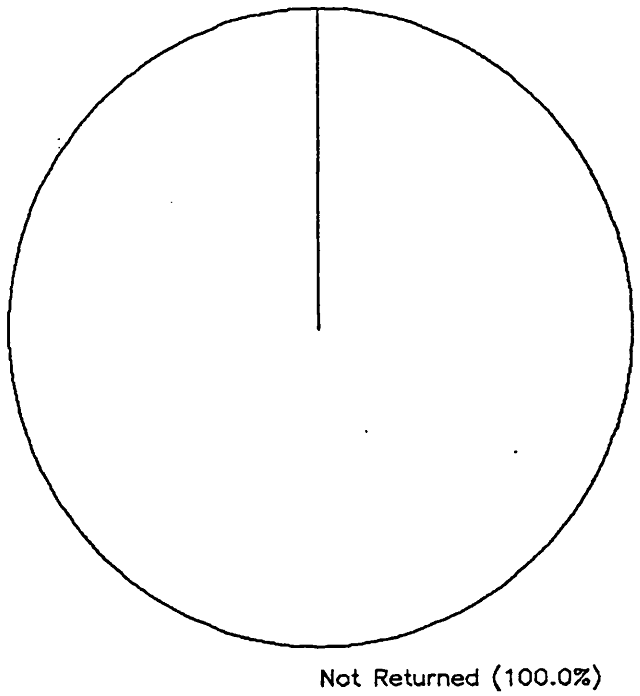


Fig A4.2: Instrument/Electrical

Questionaires

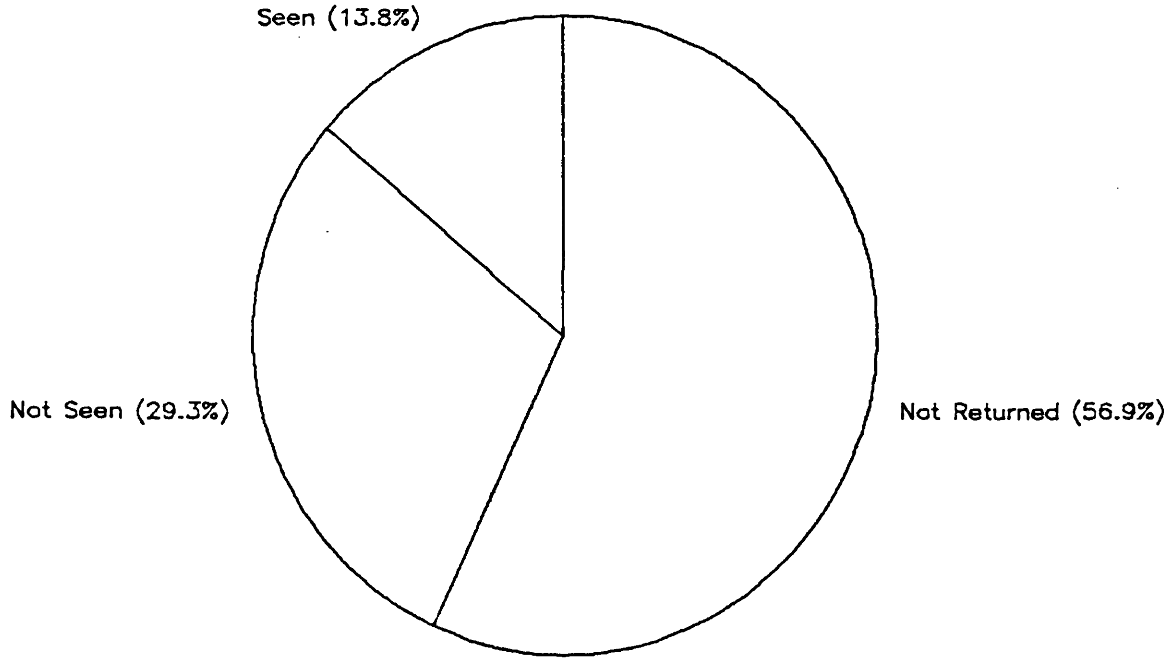


Fig A4.3: Nitric Acid

Questionaires

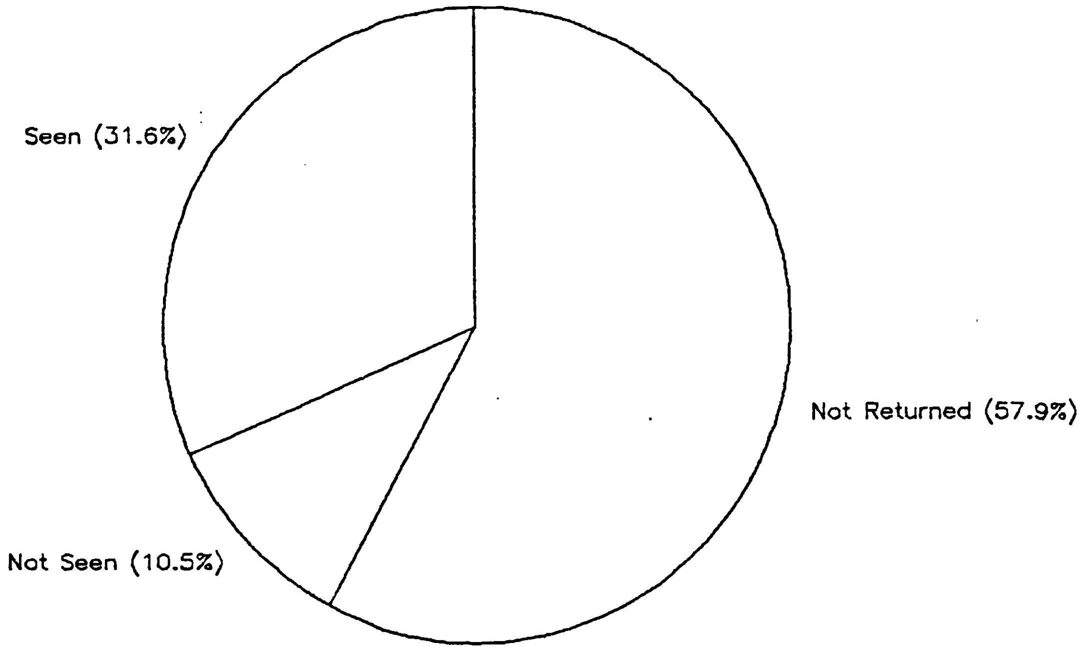


Fig A4.4: No1 Ammonia

Questionaires

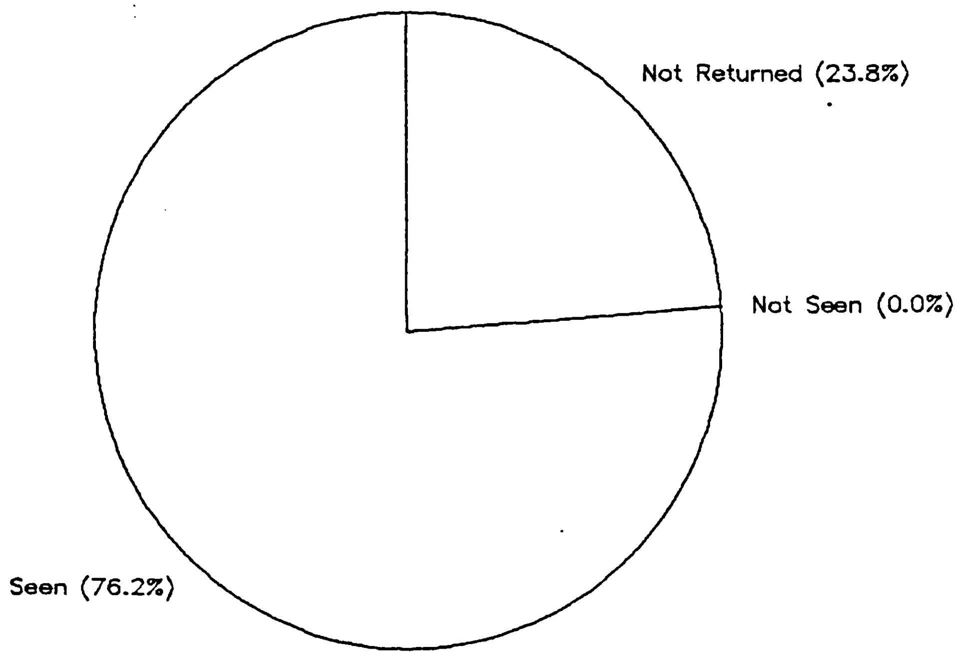


Fig A4.5: Tank Level Control

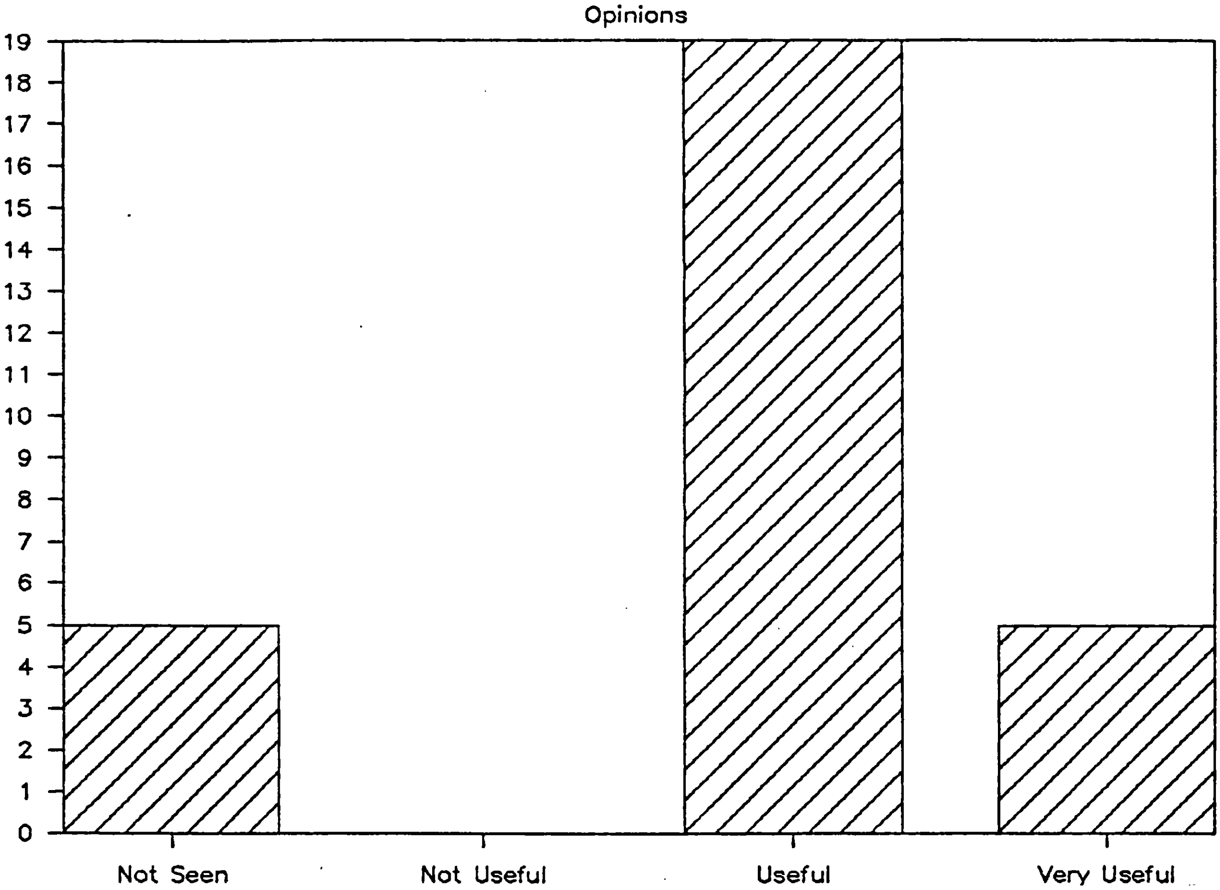
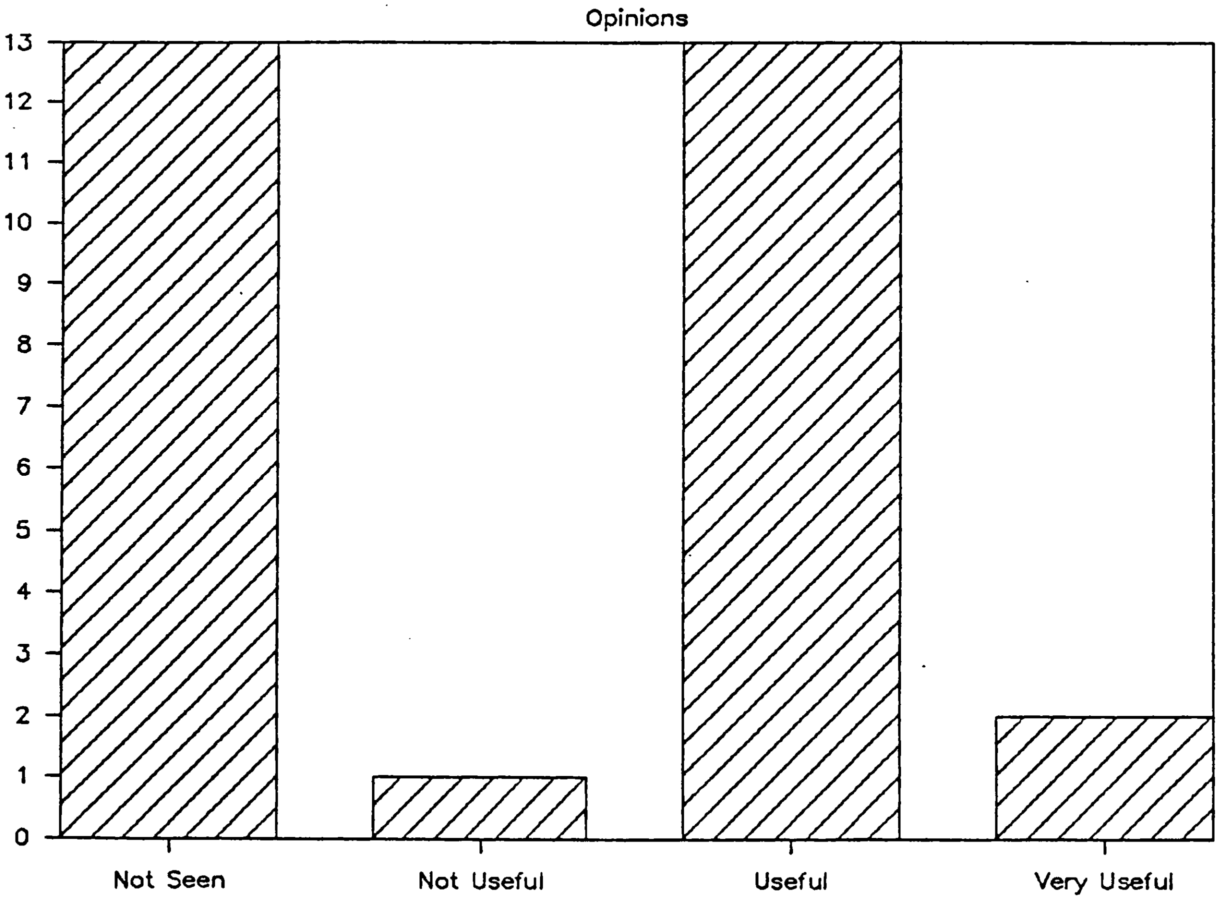


Fig A4.6: Co-Current Heat Exchanger



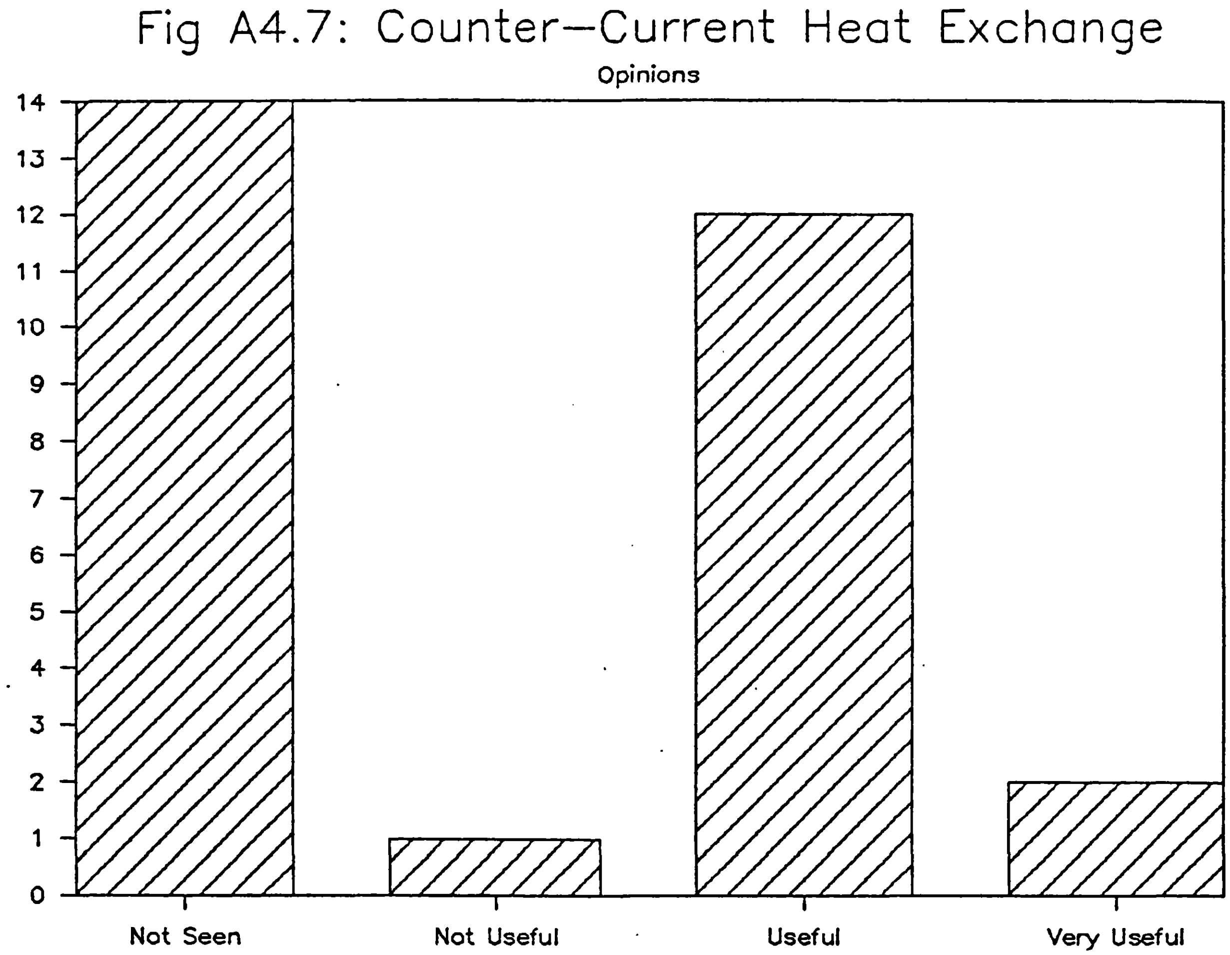


Fig A4.7: Counter—Current Heat Exchange
Opinions
14
13
12
11
10
9
8
7
6
5
4
3
2
1
0
Not Seen
Not Useful
Useful
Very Useful

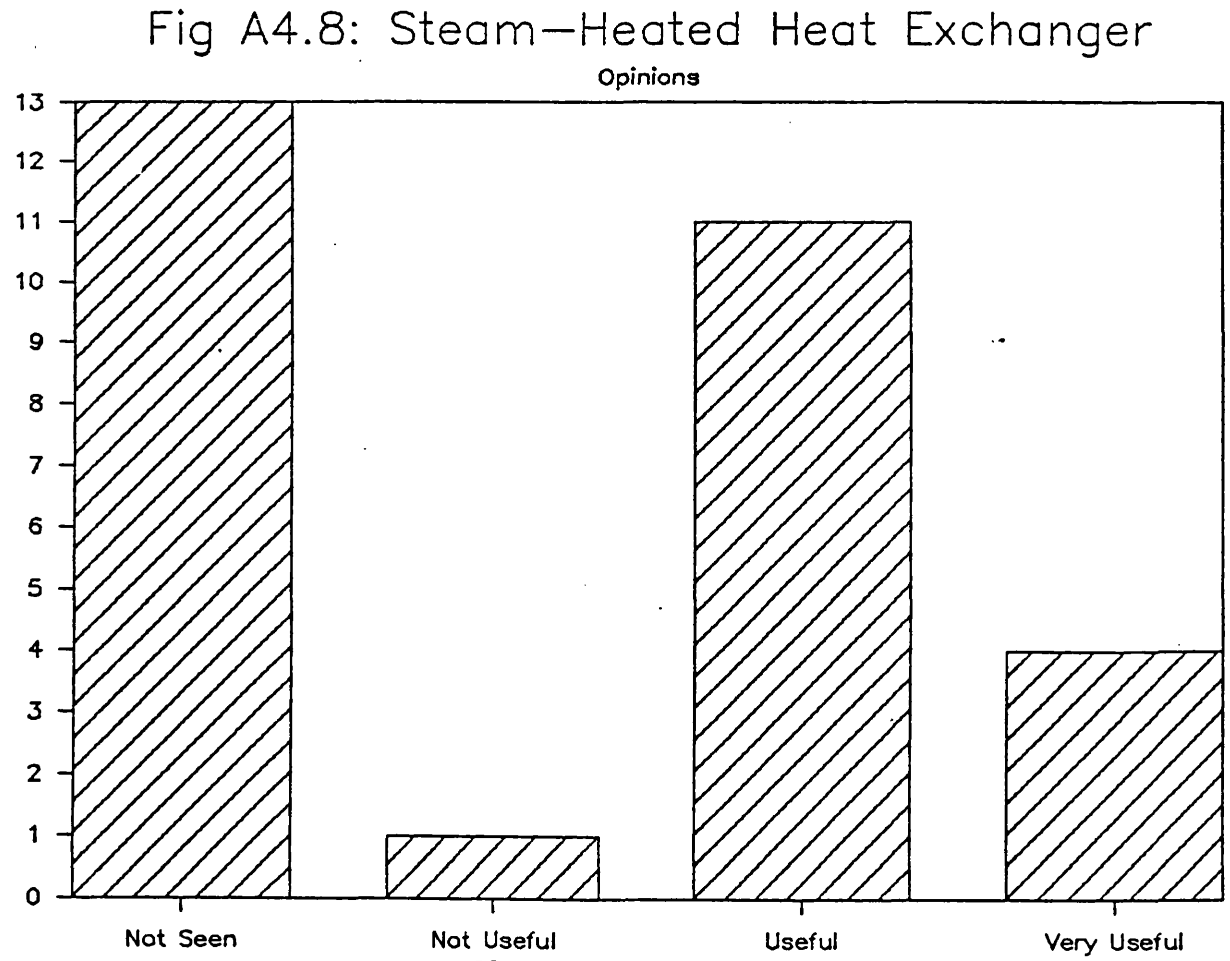


Fig A4.8: Steam—Heated Heat Exchanger
Opinions
13
12
11
10
9
8
7
6
5
4
3
2
1
0
Not Seen
Not Useful
Useful
Very Useful

Fig A4.9: Stirred Tank Reactor Control

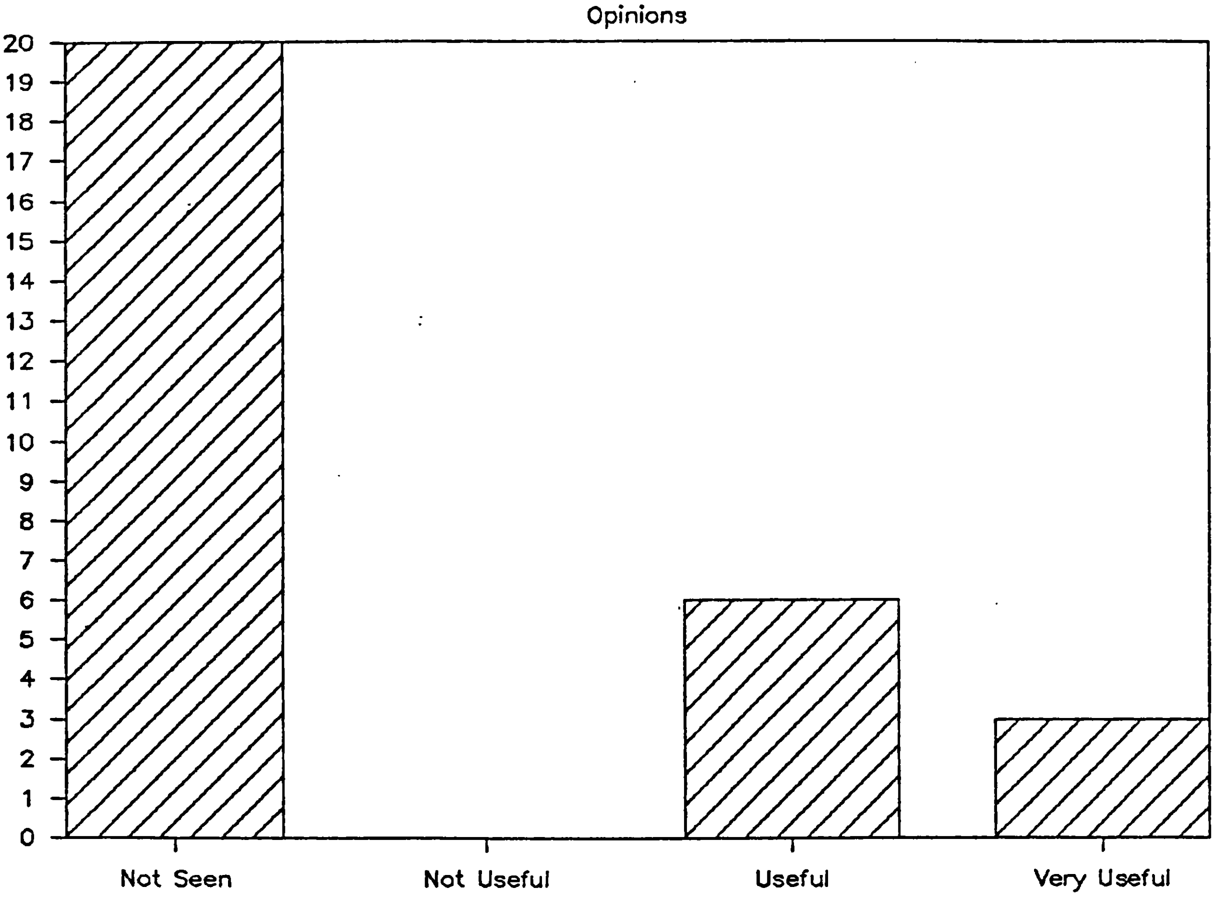


Fig A4.10: Manual By-Pass Heat Exchange

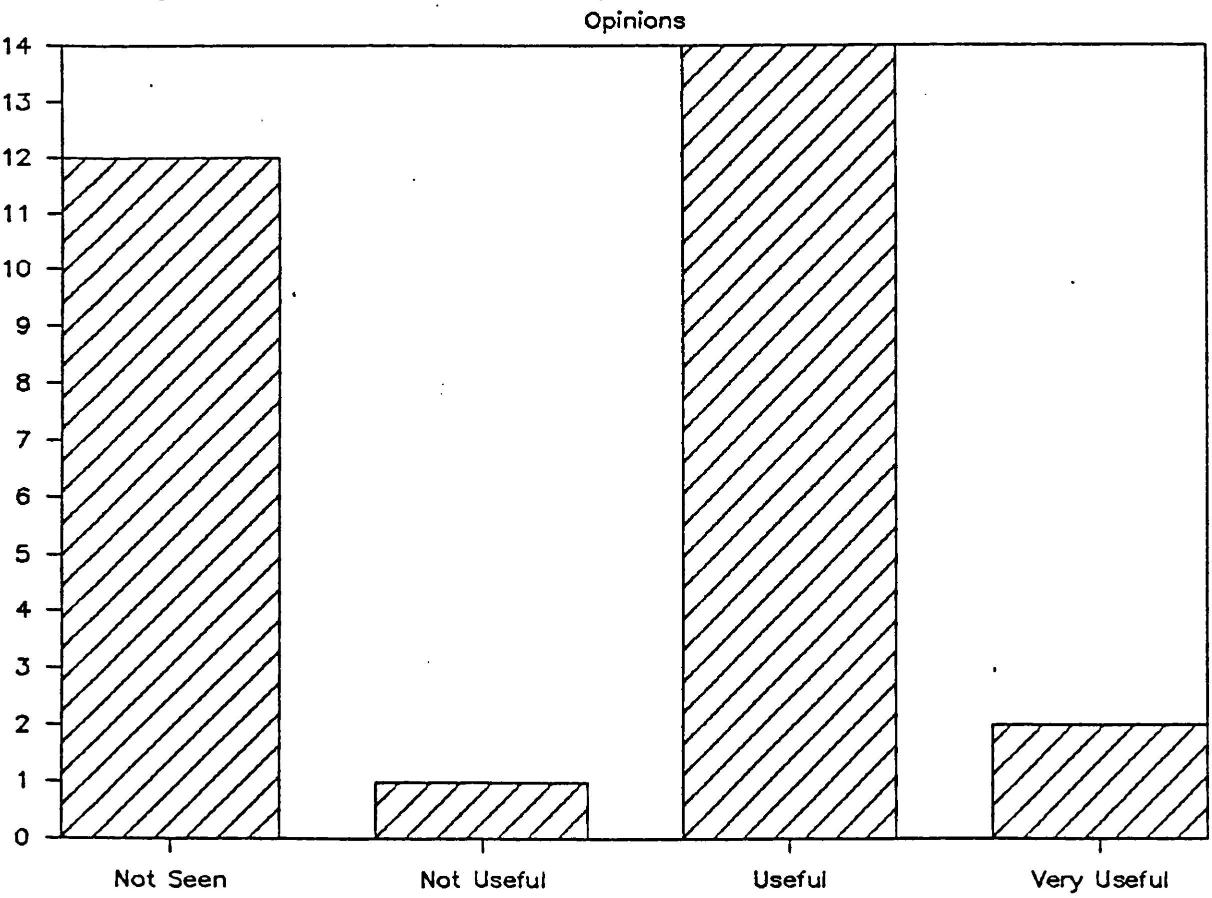


Fig A4.11: Ammonia Vaporiser Control

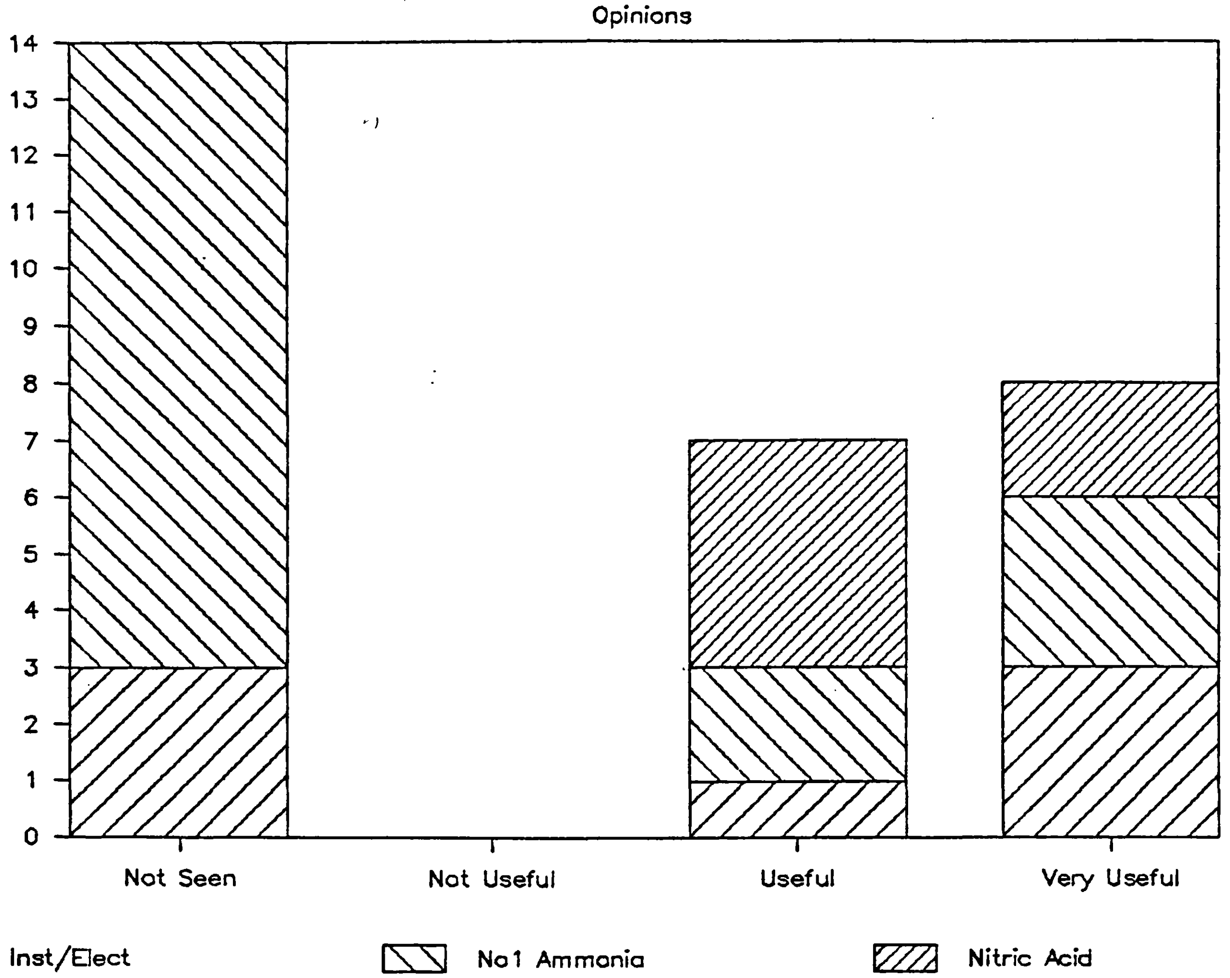


Fig A4.12: Ammonia Converter

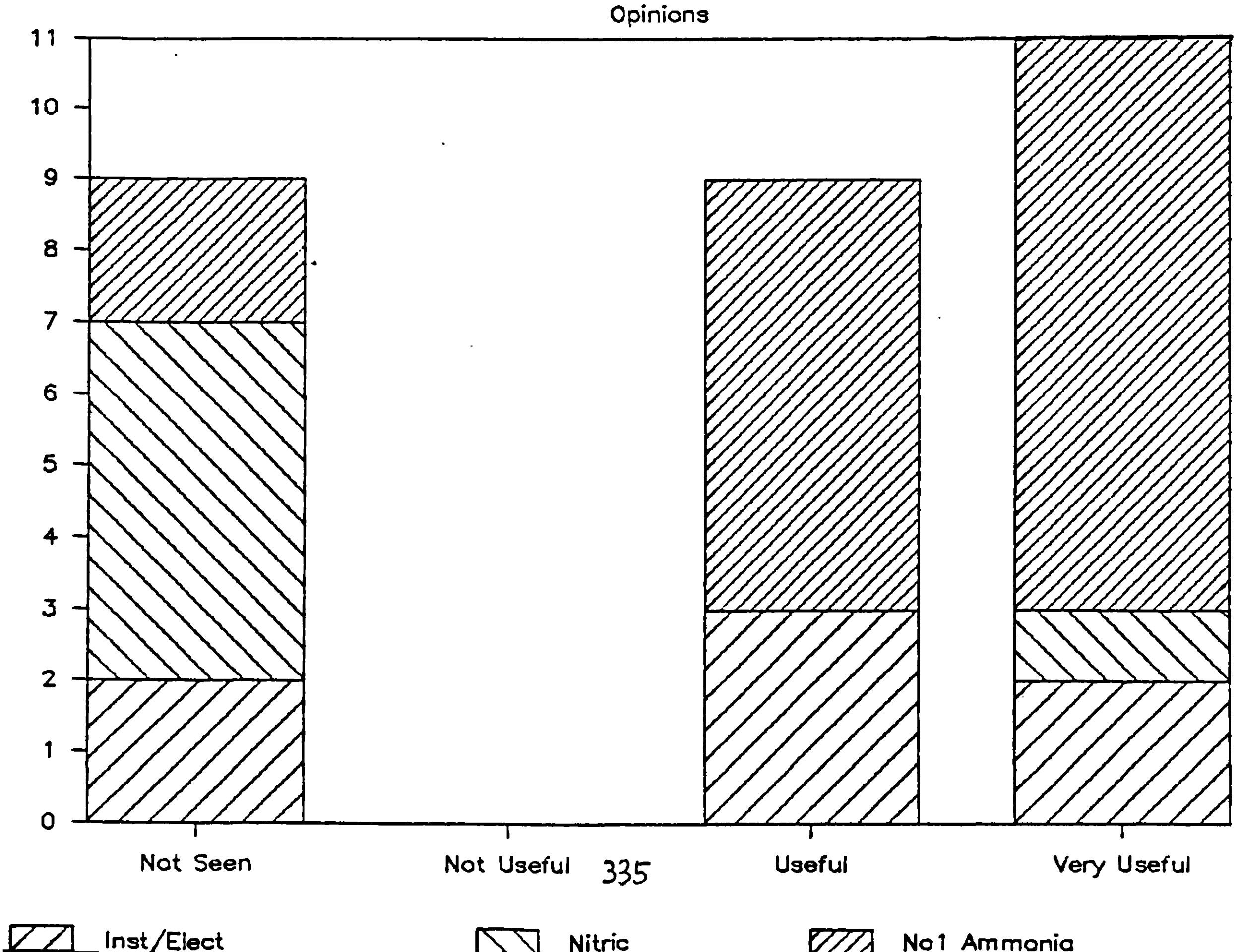


Fig A4.13: Reforming Section

Opinions

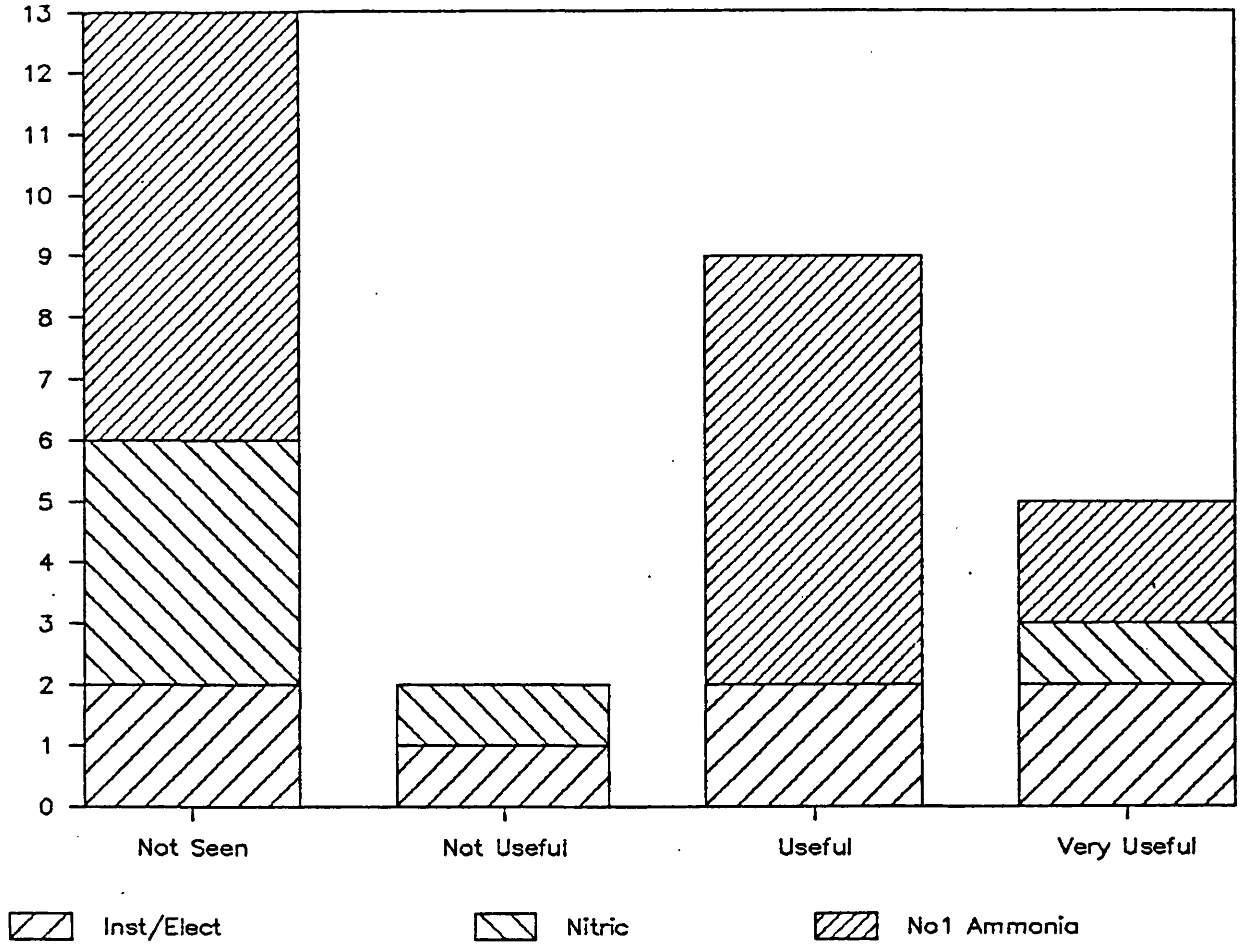


Fig A4.14: Overall Knowledge Improved

Opinions

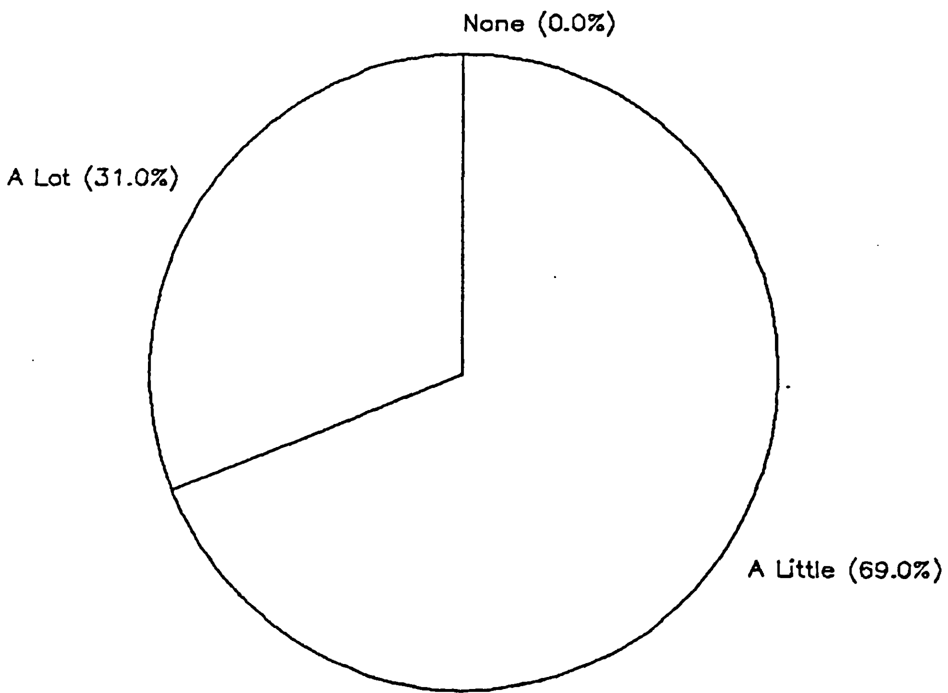


Fig A4.15: Ammonia Vaporiser Response

Opinions

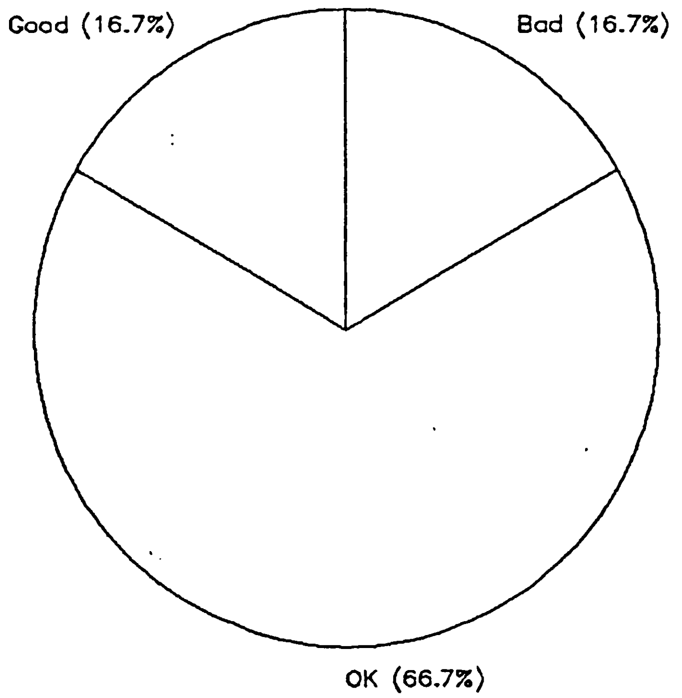


Fig A4.16: Ammonia Vaporiser Knowledge

Opinions

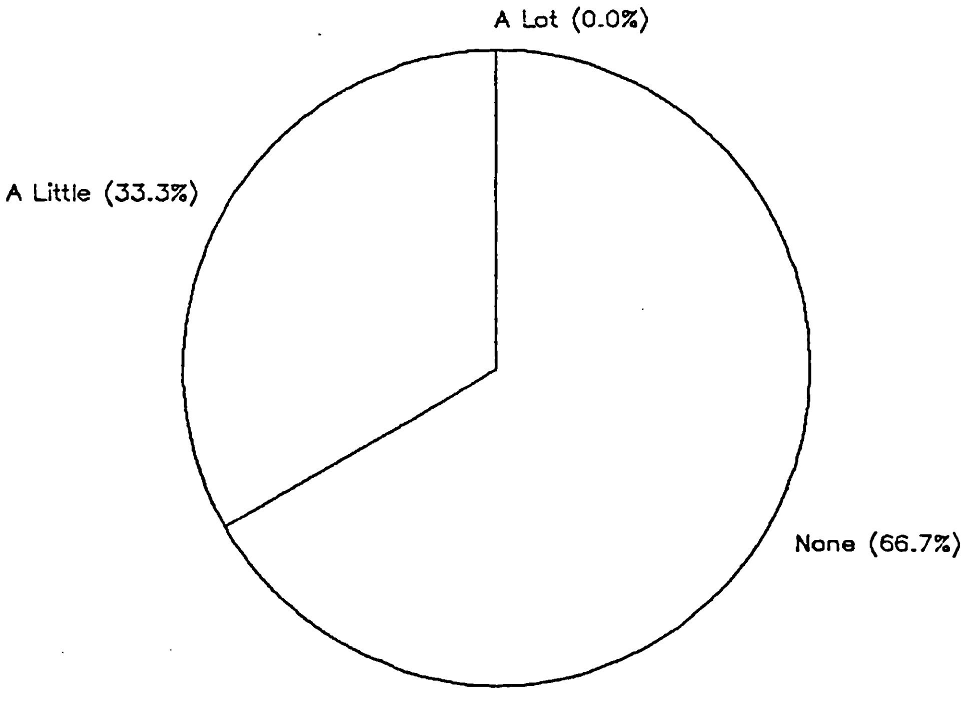


Fig A4.17: Ammonia Converter Response

Opinions

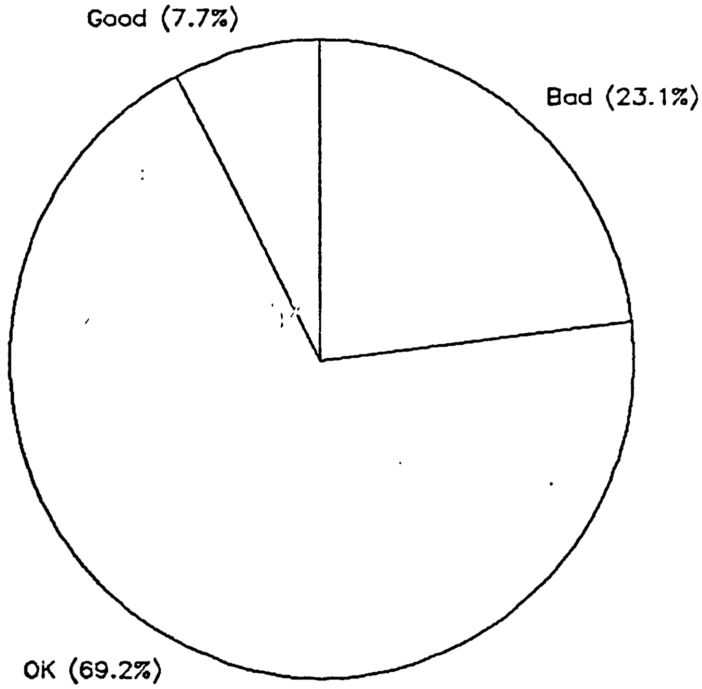


Fig A4.18: Ammonia Converter Knowledge

Opinions

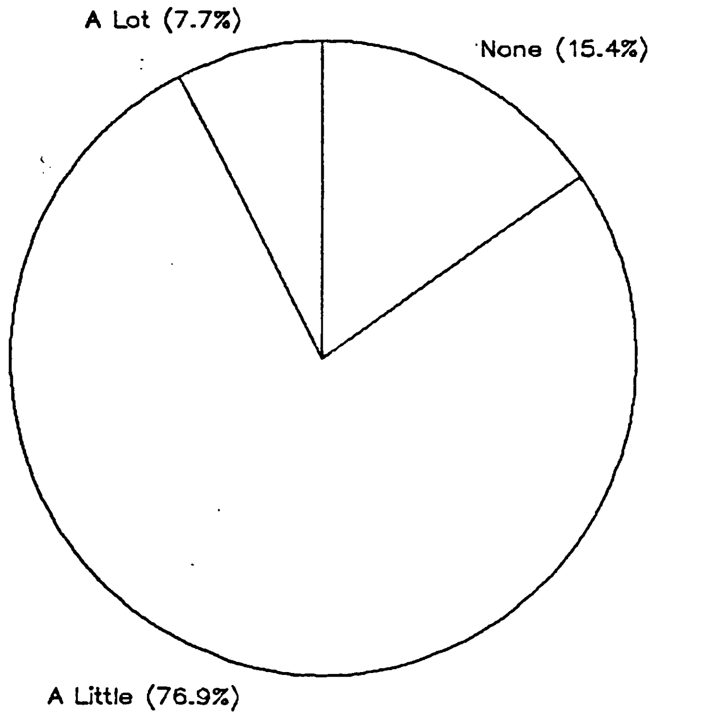
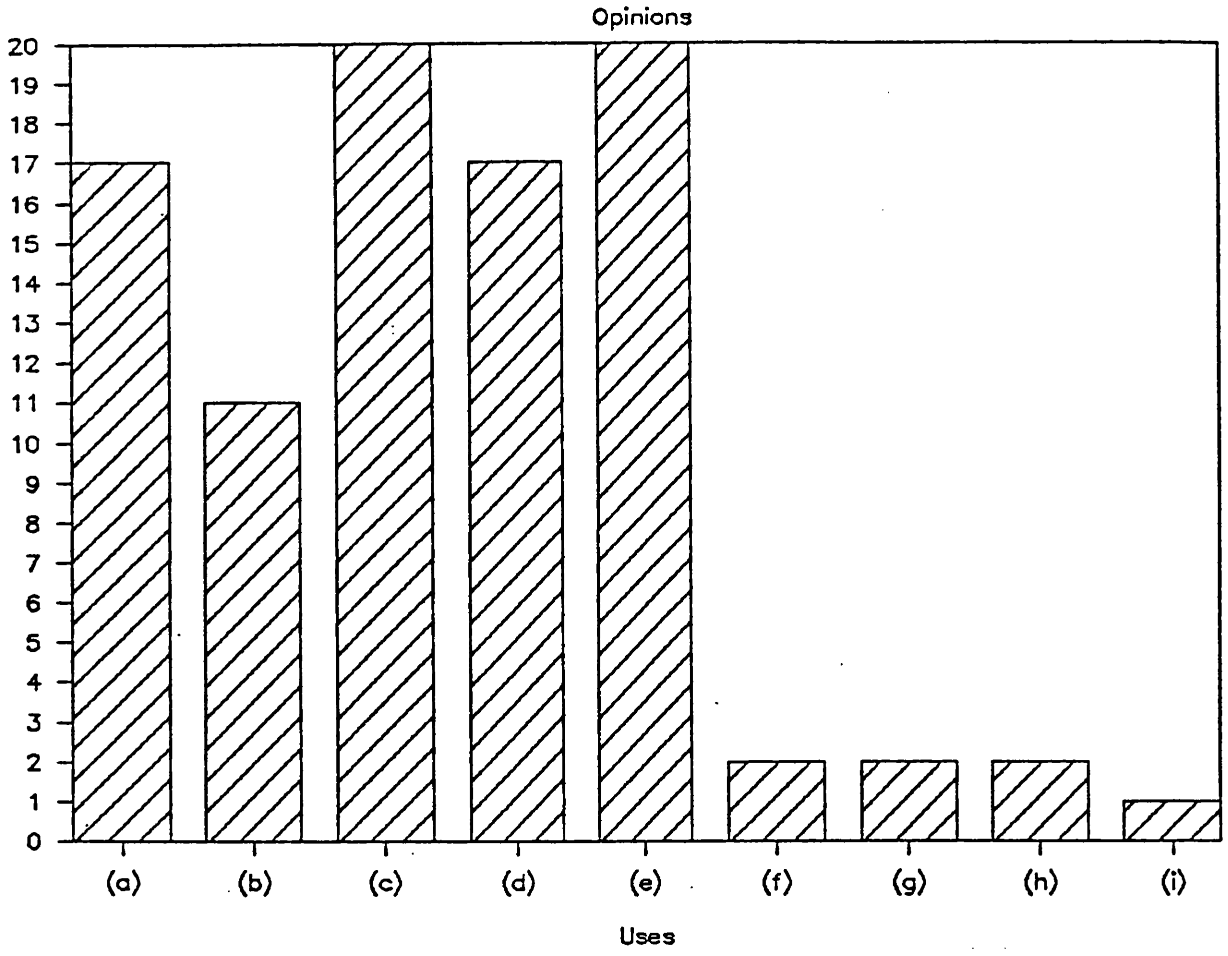


Fig A4.19: Use Of Simulations



(a) Demonstrating Faults.
(b) Demonstrating the changes in plant operating conditions due to modifications.
(c) Giving the opportunity to 'play' with the plant.
(d) Improving knowledge of plant responses.
(e) Improving knowledge of plant operation.
(f) Improving Operator confidence.
(g) Improving knowledge of other plants and so increasing flexibility.
(h) Fault finding.
(i) Livening up the Regency System !

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